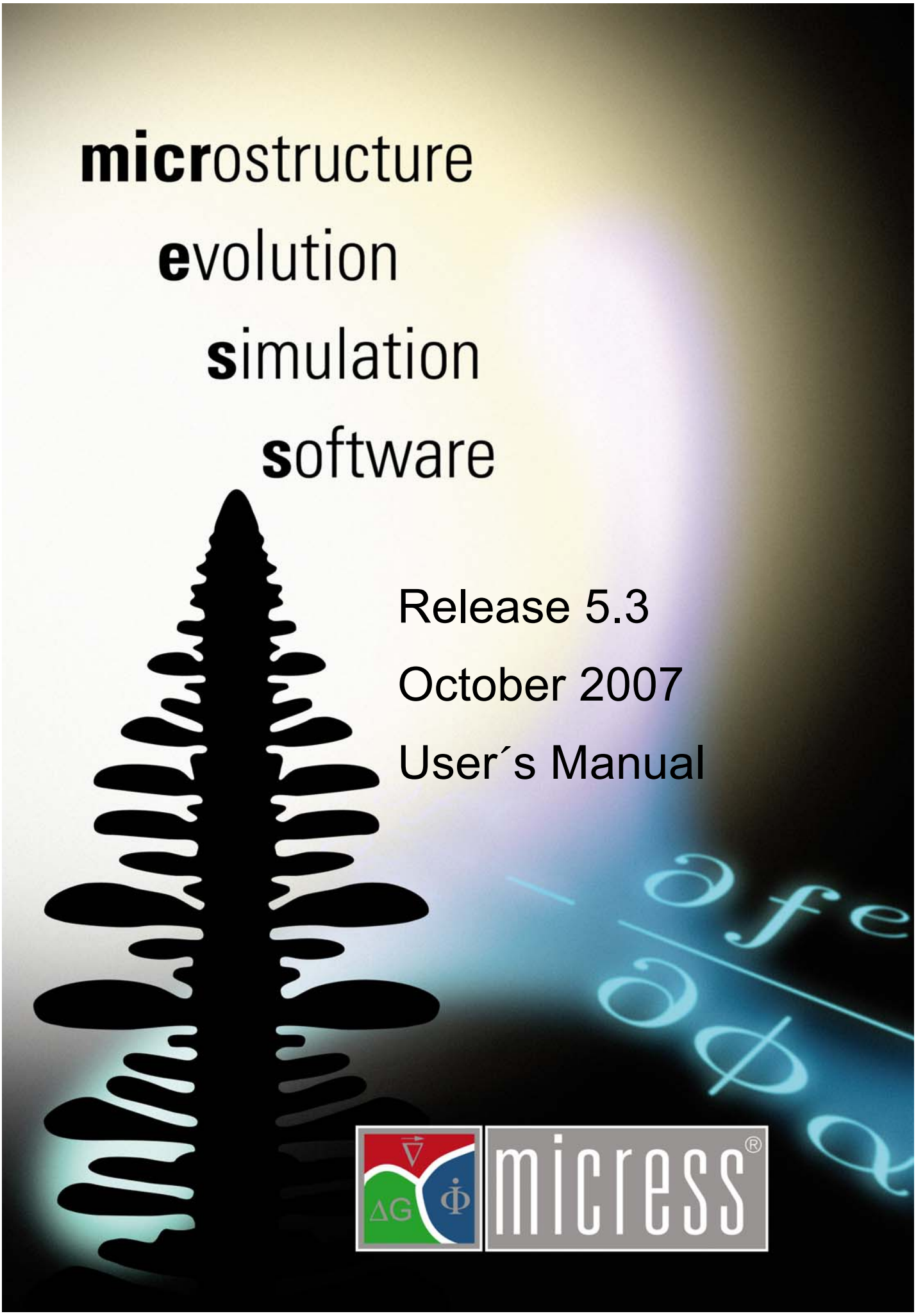
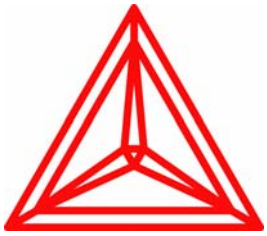

microstructure
evolution
simulation
software
Release 5.3
October 2007
User´s Manual
micress®



User Documentation

Version : V 5.3

Date : October 2007

ACCESS e.V.

Intzestr. 5, 52072 Aachen

'Resolution of partial differential equations is more about art than science'.

Apocryphal quotation from Numerical Recipes in Fortran.

'2 + 2 = 4 except for large values of 2'.

Anonymous.

'42'.

Douglas Adams.

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1 Introduction.

1.1 Scope of the software MICRESS®.

The present software MICRESS® (***MICR***ostructure ***E***volution ***S***imulation ***S***oftware) is developed for a time- and space-resolved simulation of solid-liquid and solid-solid phase transformations in metallic alloys by solving the free boundary problem of moving phase boundaries.

MICRESS is based on the multi-phase-field method which defines a phase-field parameter for each phase involved. The phase field parameter describes the fraction of each phase as a continuous function of space and time. Additionally each single grain is mapped to a distinct phase-field parameter, and formally treated as an individual phase. The theory leads then to a set of coupled partial differential equations which describes the evolution of the phase-field parameter, and concentration, temperature, stress and flow fields. (Please see Reference list in section 11.2 for some literature on that subject).

The total set of equations is solved explicitly by the finite difference method on a cubic grid.

MICRESS handles:

- 1, 2, 3 dimensional calculation domains
- arbitrary number of components, phases and grains
- solid-solid and solid-liquid interaction
- anisotropy of grain boundaries, mobility and energy
- it also supports run-time coupling to thermodynamic database (via the TQ-interface of Thermo-Calc™)

Restrictions:

- square (cubic), equally spaced grid.

1.2 Contact in case of problems.

The MICRESS® site can be visited at:

www.micress.de

It has lots of up-to-date information, and provides links to the MICRESS user forum and the MICRESS hotline web page (for which you should have been issued a user-ID and password).

Looking up the MICRESS forum should be the first step if you were to experience any difficulty, as it is most likely to have the answer to your question (chances are someone already asked the same!), if not, do not hesitate to post a message: it will be answered as soon as possible.

> *As was creatively phrased by someone who wishes to remain anonymous, "the forum is the main operating theatre of our **R**eliable **T**ask-**F**orce for **M**ICRESS® which thrives to provide **R**esponses **T**ailored **F**or **M**ICRESS®".*

2 What's new in version 5.3?

2.1 Speed enhancement

Some very noticeable improvement in speed could be achieved; the memory usage in 2D was significantly decreased.

2.2 Averaging

The algorithm for the averaging along the normal to the interface has been improved. The possibility of averaging not only along the normal itself, but also with some deviation, has been added, which helps minimising the effects of the grid anisotropy.

2.3 Curvature undercooling and nucleation

The curvature undercooling can now be taken into account when evaluating nucleation undercooling at interfaces.

2.4 Stoichiometric phases

Using stoichiometric phases has become significantly less error-prone and raises fewer numerical issues.

2.5 'Grain data' output

A new output is available, specifying for each grain and output time, the grain's number, phase number, its surface (volume in 3D), its derivative over time, the grain perimeter (surface in 3D), as well as its number of neighbours, and the list of its neighbours.

This data can readily be used to evaluate grain size distribution, or other user-defined plots.

2.6 Compressed results

MICRESS can now write compressed results: the gains depend on the type of output and the simulation, but fields which have a constant value over the bulk of a grain ('phas', 'intf', ...) get compressed down to a few percent of their original size, for the others outputs, apart from a few oddities, a gain of at least one third can be expected. The results of the 'distribution examples' were reduced down to a quarter of their original size.

2.7 Messages

The 'messages' are now 'embedded' in the executable, making sure the set corresponding to the current executable is used, and freeing the user of this external dependency.

2.8 CygWin

For the Windows users wishing to observe DP_MICRESS in its natural habitat, a CygWin (cf. www.cygwin.com) version is now available as a technology preview.

3 Installation.

Within this chapter you will find the minimal system requirements for which operation of MICRESS is approved. Section 3.2 contains information about the files being part of your MICRESS release. Section 3.3 describes the installation procedure.

3.1 System requirements.

The operation of the current version MICRESS is approved for the following minimal system configuration:

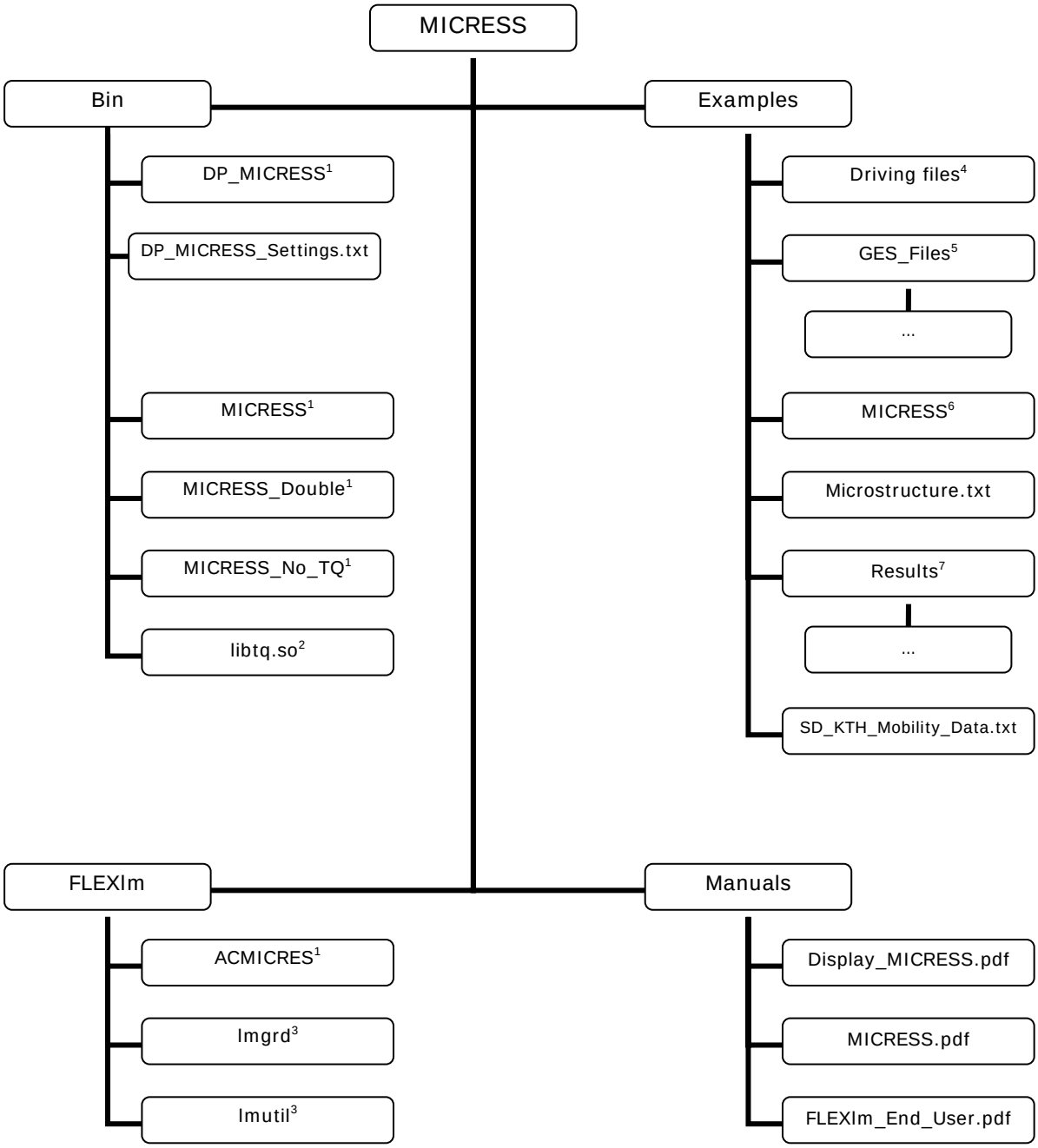
- ⇨ Windows (WinNT or higher) or Linux (version 2.2 or higher)
- ⇨ Processor Intel Pentium III (or 100 % compatible) and 512 MB main memory
- ⇨ Graphic card
- ⇨ 2 GB disk storage

3.2 Other platforms.

Standard MICRESS versions support only Windows and Linux.

3.3 MICRESS distribution files.

After installing MICRESS you should have the following files:



[1]: under Windows file name becomes "~.exe"
[2]: under Windows "tq6.dll", and "Dformd.dll"
[3]: under Windows "lmtools.exe"
[4]: several files, c.f. chapter 8, "Standard examples" for a detailed list.
[5]: there are two directories "GES_Files_Unix" and "GES_Files_Intel" (respectively for 'big-' and 'little-endian' platforms).
[6]: link to "MICRESS" binary: "MICRESS.lnk" under Windows.
[7]: several directories, c.f. chapter 8, "Standard examples" for a detailed list.

3.4 Installation Procedure.

Installing MICRESS® should be quite straightforward with its installer, please do not hesitate to contact us if you experience any difficulty. For installation under Windows™, it is highly advisable to have 'power user' privileges (i.e.: have the right to modify the registry) as file associations can then be performed by the installer itself (this nevertheless by no mean a requirement). Please see section 12 for further information on this topic.

3.5 MICRESS® license.

Special care has been given to keeping the license side of MICRESS as inconspicuous as possible; it is based on the FLEXlm™ system. Please contact your MICRESS agent if you have any doubt.

3.6 Thermo-Calc™ license.

To use MICRESS coupled to Thermo-Calc™ (via its TQ interface) requires a valid license from Thermo-Calc Software AB (www.thermocalc.se). Before trying to use MICRESS make sure your license file can be found by the license manager.

4 Running MICRESS®.

MICRESS asks for input data from the terminal by a *read* statement. More conveniently the input can be read from a text file (so called *driving file*), via a shell or directly read by the executable. Some such driving files are included in your installation directory (they are marked by *"*_dri"* or *"*_dri.txt"* under Windows). These files contain all the necessary input for MICRESS.

4.1 Preparing the input data (pre-processing).

All necessary input data must be defined in the driving file, for example control information for data output, definition of the initial state, such as position and size of initial grains or the material parameters, like phase diagram information, or diffusion data. In the next chapter one example driving file is discussed more extensively.

Driving File

```
                                                    ...
#
# Name of output files                                  Specify here the path and generic
# ==============                                        name for output files
# Name of result files?
Results_Gamma_Alpha/Gamma_Alpha
# Overwrite files with the same name?
# Options:   overwrite     write_protected    append
#            [zipped|not_zipped]            [unix|windows|non_native]
overwrite
#
#
# Selection of the outputs
# ================
# Restart data output?                          ('rest')
# Options:    out_restart     no_out_restart       [wallclock time, h.]
out_restart
# Grain number output?                           ('korn')
# Options:    out_grains      no_out_grains                Select here (by setting to '*no_*') the
out_grains                                                 outputs *not* to be written out
# Phase number output?                           ('phas')
# Options:    out_phases      no_out_phases        [no_interfaces]
out_phases
# Fraction output?                              ('frac')
# Options:    out_fraction    no_out_fraction      [phase number]
no_out_fraction
# Average fraction table?                        ('TabF')
# Options:    tab_fractions   no_tab_fractions     [front_temperature]
tab_fractions
# Interface output?                             ('intf')
# Options:    out_interface   no_out_interface     [sharp]
out_interface
# Driving-force output?                          ('driv')
# Options:    out_driv_force  no_out_driv_force
out_driv_force
# Interface mobility output?                      ('mueS')
# Options:    out_mobility    no_out_mobility
no_out_mobility

                                                    ...
```

4.2 Start the calculation.

Under UNIX type the name of the MICRESS® binary followed by the driving file, MICRESS will then parse its contents.

Under Windows, 'drag and drop' the driving file on the MICRESS® binary (or a link to it), or use the contextual menu (which should have been made available by the installer) by right-clicking the driving file (which should have a ".txt" extension).

4.3 Check the output.

During run-time, some information can be read on screen: first the input data is displayed as the same time as it is read by MICRESS, then during calculation time, other data can be read, such as the current time-step and the temperature at the bottom of the calculation along with processing-time. Also, each time a new phase or grains appears the user can be notified.

The output of MICRESS consists of various files, whose content is specified by the extension:

- **.log* is the log file of simulation-time output (in ASCII).
- **.in* is the driving file created by MICRESS (which can be used to repeat the simulation).
- **.geoF* stores information relative to the geometry (i.e.: grid size, cell dimension).
- **_TQ.txt* (Windows specific) stores: the output of Thermo-Calc™´s TQ interface which makes it more convenient to see the text of TQ 'fatal' errors

Please see section describing the Outputs for an exhaustive overview of the output files written by MICRESS.

Windows naming conventions: *MICRESS* Windows version creates file names in a slightly different way: the previous extensions are appended to the simulation name with an underscore, and then followed by '*.mcr*' for binary files and '*.txt*' for ASCII files to be able to make use of Windows' file association features. For example the UNIX file *'Simulation.log'* becomes *'Simulation_log.txt'* and *'Simulation.phas' 'Simulation_phas.mcr'*. The conversion tool from Display MICRESS can also rename the files once the simulation has been completed.

5 Driving files.

MICRESS inputs are read from a text file (so called ‘driving file’), which is actually quite convenient to perform similar simulations.

Attention should also be paid to the on-screen information when starting new simulations from scratch as significant hints are provided by MICRESS on which values they should be set to.

The driving files are divided into several sections which are: Language settings, Dimension parameters, Restart, Outputs, Time input data, Phase data, Grain input data, Nucleation parameters, Phase interaction data, Diffusion data, Phase diagram data, Initial concentrations, Elastic material data, Latent heat parameters, Temperature data, and Boundary conditions.

5.1 ‘Switching’ to keyboard input.

When making modification to a driving file, it is sometimes convenient to make the input for a ‘block of settings’ interactively (for example, when one is not sure about the exact sequence of the input expected by MICRESS®). This can be achieved by inserting the keyword “__*Switch*__” in the driving which causes subsequent input to be read from the keyboard, typing this keyword again at any later time makes MICRESS® revert to file input for further input. (The user should make sure that the contents of driving file correspond to the input expected by MICRESS®: processing of the driving file is simply resumed after the keyword).

5.2 MICRESS License.

MICRESS looks up whether a valid license can be found at several default locations: previously valid licenses found (if any!), working directory (directory where the binary is under Windows), a license server is running on the local machine (under UNIX), or the file (or machine) specified by the 'MICRESS_LICENSE' environment variable. If no valid license can be found in this way, the user will be prompted for it: this only has to be done once, as the locations of the valid licenses are ‘remembered’ by FLEXlm.

MICRESS on-screen output

```
...
#
# License
# =====
# No valid license could be found at the default locations:
#  working directory, 'localhost' and
#  file specified by the  'MICRESS_LICENSE' environment variable
# Please specify a license file
#  or a machine where a license server is running
...
```

5.3 Language settings.

In the section, the language settings have to be defined, the first being the chosen language (MICRESS supports English, French and German).

Driving File

```
...
#
# Language settings
# ============
# Please select a language: 'Deutsch', 'English' or 'Francais'
English
#
...
```

5.4 Dimension parameters.

First parameters related to the dimensionality are set: the domain, in number of cells in each direction, and the grid spacing (in µm). For 2D calculations: AnzY=1, for 1D calculations: AnzX=1, AnzY=1.

Then various flags have to be selected: first the type of coupling, which can be one of the following: *'phase'* (i.e.: no coupling, pure phase-field), *'concentration'*, *'temperature'*. *'temp_cyl_coord'* is a special option which calculates a 2D temperature field in a cylindrical coordinate system. In addition *'stress'* and *'stress_coupled'* can be specified in the same line, activating the calculation of the elastic stress field and the coupling to the phase field equation, respectively. So far, it only works with concentration coupling. The phase-field potential function also has to be chosen: '*double_obstacle'* or '*double_well'*. The averaging of the driving force along the normal to the interface can be toggled on and off with '*averaging'* and 'no*_averaging'*. Similarly in the case of concentration coupling, one dimensional far field approximation for solute

Driving File

```
...
# Flags and settings
# ============
#
# Geometry
# -----------
# Grid size?
# (for 2D calculations: AnzY=1, for 1D calculations: AnzX=1, AnzY=1)
# AnzX:
250
# AnzY:
1
# AnzZ:
250
# Cell dimension (grid spacing in micrometers):
0.25000000
#
# Flags
# ------
# Type of coupling?
# Options:    phase  concentration  temperature  temp_cyl_coord
#           [stress]  [stress_coupled]  [flow]
concentration
# Type of potential?
# Options:    double_obstacle    double_well
double_obstacle
# Enable averaging of the driving force along the normal to the interface?
# Options:    averaging    no_averaging
averaging
# Enable one dimensional far field approximation for diffusion?
# Options:    1d_far_field    no_1d_far_field
no_1d_far_field
# Shall an additional 1D field be defined in z direction
# for temperature coupling?
# Options:    no_1d_temp  1d_temp  1d_temp_cylinder  1d_temp_polar
no_1d_temp
#
# Phase field data structure
# ----------------------------
# Coefficient for initial dimension of field iFace
#  [minimum usage] [target usage]
0.1
# Coefficient for initial dimension of field nTupel
#  [minimum usage] [target usage]
0.1
#
...
```

diffusion can enabled with '*1d_far_field*' (or '*no_1d_far_field*'), when activated the user is asked for the length (in cells) of the '1D external extension' (purely 1D extension to the domain which can be used to resolve long concentration profile without having to increase the calculation domain itself unduly), and additional files describing the concentration profiles *outside* of the domain will be created (the '1D_Ext' files previously mentioned).

Afterwards the user is prompted for data structure parameters: the initial dimension of field *IFace* (used to store data related to the interface points), as a fraction of AnzX × AnzY × AnzZ, and of the field *nTupel* (for higher-order junctions), input in a similar way. These are initial dimensions and the corresponding arrays are fully dynamic, so the influence of these parameters is now quite limited, but they can nevertheless be fine-tuned if need be via two additional parameters: the 'minimal' and 'target' usage. With the "0.25 0.75 0.50" setting, the lists will start with dimension of one fourth of AnzX × AnzY × AnzZ, and should they be re-allocated (because they are too short, or too long, see afterwards), they would afterwards be 75 % full, also should less than 50 % of them be used they would also be resized (also so that they are three-quarter full).

Driving File

```
...
# Phase field data structure
# --------------------------
# Coefficient for initial dimension of field iFace
#  [minimum usage] [target usage]
0.25   0.75   0.50
# Coefficient for initial dimension of field nTupel
#  [minimum usage] [target usage]
0.10   0.75   0.50
#
...
```

5.5 Restart.

The user has to specify if he wishes to restart a previous simulation or begin a new one. Even if a simulation is restarted all input parameters have to be specified, so as to leave open the opportunity of modifying them.

Note: extreme caution should be exercised when modifying dimension parameters in conjunction with the restart feature.

Driving File

```
...
#
# Restart options
# ==========
# Restart using old results?
# Options:   new      restart
new
#
...
```

5.6 Output name.

The ‘base name’ of the results is to be specified next: the name each output file will be derived from it, under Linux, by appending an extension identifying the contents of the file (see next section). Under Windows, the principle is the same, though the marker identifying the contents of the file is rather appended to the ‘generic’ name after an underscore, followed by an *.mcr*' for binary files and '*.txt*' for ASCII files.

Driving File

```
                                        …
#
# Name of output files
# ==============
# Name of result files?
Results_Gamma_Alpha/Gamma_Alpha
# Overwrite files with the same name?
# Options:   overwrite     write_protected     append
#              [zipped|not_zipped]              [unix|windows|non_native]
overwrite
                                        …
```

For example, when specifying ‘Simulation’ as a ‘base name’ under Linux leads to outputs named ‘Simulation.log’ and ‘Simulation.geoF’, whereas under Windows™ they would be called ‘Simulation_log.txt’ and ‘Simulation_geoF.mcr’.

Additionally, ‘*Gesamt’* result files (denoted by ‘G’) and / or ‘1D extension’ (marked with ‘1D_Ext’), as well as ‘1D temperature’ (‘1D_Temp’) can also be created. The output files *G.* are created for simulations with a moving calculation domain (see the section related to Boundary conditions)., they hold the information for the accumulated domain including the areas which are moved out from the actual calculation frame. The ‘1D_Ext’ files store the composition in the 1D extension of the concentration field (please see Dimension parameters). The ‘1D_Temp’ output are related to the one-dimensional external temperature field (see also Dimension parameters).

The next output specify how should file which would possibly have the same name be dealt with: MICRESS can try to overwrite them without any warning (if the operating system allows the user to do it), or an error can be issued. In combination with restart, it is also possible to append to files with the same name.

It is also possible to specify whether the default naming scheme (i.e.: Linux or Windows™) should be overridden (for examples for users running simulations under Linux, but post-processing the results under Windows). Similarly, for completeness, it is also possible *not* to compress the binary outputs.

5.7 Outputs.

In this section, the user can select the outputs which are going to be written out. Here is a comprehensive overview of all files that can be written out by MICRESS, unless otherwise specified these binary files to be viewed with DP_MICRESS. Similarly, unless otherwise specified these files are updated at the user-requested outputs time described in the following section, rather than as *'tab_log'* outputs (see hereafter). (All files are listed here in alphabetical order of the 'extension'):

- **.concN* for the concentration of component N (when the concentration coupling is activated and *'out_conc'* is not set to *'no_'*). The concentrations are in at% or wt% (as set in the driving file).
- **.cPhaN* is similar to the previous output, except in the interface regions, where the concentration in a given phase is given out (as opposed to the mixture concentration), it is written out when the concentration coupling is activated and *'out_conc_phase'* is not set to *'no_'*.
- **.dGsp* for the contribution of stress to the driving force (for *'stress_coupled'* simulations and *'out_dG_stress'* is not set to *'no_'*), in J/cm^3.

Driving File

```
                                        ...
#
# Selection of the outputs
# ================
# Restart data output?                          ('rest')
# Options:    out_restart     no_out_restart      [wallclock time, h.]
out_restart
# Grain number output?                          ('korn')
# Options:    out_grains      no_out_grains
out_grains
# Phase number output?                          ('phas')
# Options:    out_phases      no_out_phases       [no_interfaces]
out_phases
# Fraction output?                              ('frac')
# Options:    out_fraction    no_out_fraction     [phase number]
no_out_fraction
# Average fraction table?                       ('TabF')
# Options:    tab_fractions   no_tab_fractions    [front_temperature]
tab_fractions
# Interface output?                             ('intf')
# Options:    out_interface   no_out_interface    [sharp]
out_interface
# Driving-force output?                         ('driv')
# Options:    out_driv_force  no_out_driv_force
out_driv_force
# Interface mobility output?                    ('mueS')
# Options:    out_mobility    no_out_mobility
no_out_mobility
# Curvature output?                             ('krum')
# Options:    out_curvature   no_out_curvature
no_out_curvature
# Interface velocity output?                    ('vel')
# Options:    out_velocity    no_out_velocity
no_out_velocity
# Should the grain-time file be written out?    ('TabK')
# Options:    tab_grains      no_tab_grains       [extra|standard]
tab_grains
# Should the 'von Neumann Mullins' output be written out?   ('TabN')
# Options:    tab_vnm   no_tab_vnm
no_tab_vnm
# Should the 'grain data output' be written out?    ('TabGD')
# Options:    tab_grain_data   no_tab_grain_data
no_tab_grain_data
# Temperature output?                           ('temp')
# Options:    out_temp        no_out_temp
no_out_temp
# Concentration output?                         ('conc')
# Options:    out_conc        no_out_conc         [list of comp.]
out_conc
# Concentration of reference phase output?      ('cPha')
# Options:  out_conc_phase  no_out_conc_phase   [phase nb.] [l. of c.]
no_out_conc_phase
# Average concentration per phase (and extrema)?    ('TabC')
# Options:    tab_conc      no_tab_conc
no_tab_conc
                                        ...
```

- **.dTLat* for the intermediate data relative to the release of latent heat (when the concentration coupling is activated and *'lat_heat'* is not set to *'no_'*), in ASCII format.
- **.diff*: shows the data provided by Thermo-Calc™ via its TQ interface for the diffusion coefficients, in ASCII format, available when this option is activated.
- **.driv*: driving force for growth of grain with higher number into the lower one (when *'out_driv_force'* is not set to *'no_'*), in J/cm^3.
- **.frac* for the fraction of solid (when *'out_fraction'* is not set to *'no_'*), similarly **.fracN* shows the fraction of phase N.
- **.geoF* stores information relative to the geometry (i.e.: grid size, cell dimension).
- **.hStr* for hydrostatic stress (when the stress coupling is activated and *'out_vMiese_stress'* is not set to *'no_'*), in MPa.
- **.in* is the driving file created by MICRESS (which can be used to repeat the simulation). This is obviously an ASCII file.
- **.intf* for tracking the interface (when *'out_interface'* is not set to *'no_'*).
- **.korn*: for the grains field (when *'out_grains'* is not set to *'no_'*).
- **.krum*: for the interface curvature (when *'out_curvature'* is not set to *'no_'*), in µm^{-1}.
- **.log* is the log file of simulation outputs (in ASCII).
- **.millx, *.milly,* and **.millz* : for the respective Miller indices (when *' out_miller'* is not set to *'no_'*).
- **.mueS*: for the local interface mobility (when *'out_mobility'* is not set to *'no_'*), in cm^4/(Js).
- **.orie* stores the grain orientation (when *'out_orientation'* is not set to *'no_'*), in 2D, in degrees.
- **.phas* for the phases information (when *'out_phases'* is not set to *'no_'*).
- **.rest* contains data necessary to restart a simulation (when *'out_restart'* is not set to *'no_'*): this binary file is not meant for internal use by MICRESS and cannot be post-processed.
- **.rex* for the stored energy (when *'out_recrystall'* is not set to *'no_'*), in J/cm^3.
- **.sxxCV, *.sxyCV, *.sxzCV, *.syyCV, *.syzCV* and **.szzCV*: components of the stress tensor, xxCV, (yyCV), zzCV are the diagonal elements in the 2D (3D) case, sxyCV, sxzCV, syzCV are off-diagonal terms (torsion), respectively (when the stress coupling is activated and *'out_normal_stress'* is not set to *'no_'*), in MPa.
- **.TabC* for the average and extrema of concentration in each phase (when the concentration coupling is activated and *'tab_conc'* is not set to *'no_'*), in ASCII format.

Driving File

```
...
# Recrystallisation output?                    ('rex')
# Options:    out_recrystall   no_out_recrystall
no_out_recrystall
# Recrystallysed fraction output?              ('TabR')
# Options:    tab_recrystall   no_tab_recrystall
no_tab_recrystall
# Miller-Indices output?                       ('mill')
# Options:    out_miller      no_out_miller
no_out_miller
# Orientation output?                          ('orie')
# Options:    out_orientation  no_out_orientation
no_out_orientation
# Should the orientation-time file be written out?    ('TabO')
# Options:    tab_orientation  no_tab_orientation
no_tab_orientation
# Should monitoring outputs be written out?          ('TabL')
# Options:    tab_log [simulation time, s] [wallclock time, min]  no_tab_log
tab_log 0.25
#
...
```

- **.TabD* gives the diffusion coefficients at the corresponding '*tab_log*' times (when the concentration coupling is activated and *'tab_log'* is not set to *'no_'*), in ASCII format.
- **.TabF* for the average fraction of each phase in the whole domain (when the concentration coupling is activated and *'tab_fractions'* is not set to *'no_'*), in ASCII format.
- **.TabGD* gives some assorted data about each grain (when *'tab_grain_data'* is not set to *'no_'*), in ASCII format.
- **.TabK*: number of grains (when *'tab_grains'* is not set to *'no_'*), in ASCII format. This file is updated by default each time a grain is set or disappears.
- **.TabL*: monitoring outputs (when *'tab_log'* is not set to *'no_'*), which are generated at user-defined intervals to check the simulation progress, it also contains additional information dependant on the type of coupling activated, in ASCII format.
- **.TabN* stores data relevant for making 'Von Neumann – Mullins plots' (when *'tab_vnm'* is not set to *'no_'*), in ASCII format.
- **.TabR* for the recrystallized fraction (when *'tab_recrystall'* is not set to *'no_'*), in ASCII format.
- **.TabO* for orientation information (when *'tab_orientation'* is not set to *'no_'*), in ASCII format.
- **.TabT* reports information relative to the setting of the (automatic) time-step (when automatic time-stepping has been selected and *'tab_log'* is not set to *'no_'*), in ASCII format.
- **.temp* for the temperature in Kelvin (when the temperature coupling is activated and *'out_temperature'* is not set to *'no_'*).
- **_TQ.txt* (Windows specific) stores: the output of Thermo-Calc™´s TQ interface which makes it more convenient to see the text of TQ 'fatal' errors. This file is always created under Windows when Thermo-Calc™ -coupling is activated.
- **.uxCV, *.uyCV,* and **.uzCV*: normal displacements (when the stress coupling is activated and *'out_normal_displacement'* is not set to *'no_'*), in percent.
- **.vel* for the interface velocity (when *'out_velocity'* is not set to *'no_'*), in µm/s.
- **.vxCV, *.vyCV, *.vzCV, *.syyCV, *.syzCV* and **.szzCV*: components of the stress tensor, xxCV, (yyCV), zzCV are the diagonal elements in the 2D (3D) case, sxyCV, sxzCV, syzCV are off-diagonal terms (torsion), respectively (when the stress coupling is activated and *'out_normal_stress'* is not set to *'no_'*), in MPa.
- **.vM* for the van Mises stress (when the stress coupling is activated and *'out_vMiese_stress'* is not set to *'no_'*) in MPa.

5.8 Time input data.

The times of user-defined intermediate outputs is to be specified here. It is sometimes convenient to have an early output just to check that the simulation has indeed normally started. Series of output with a regular interval can be easily input with *'linear_step' or 'logarithmic_step'*, which prompts for an increment and the end value: on the previous example, the user request outputs for t = 00.25 s, 01.00 s, every 00.50 s until 10.00 s, and every 01.00 s until 25.00 s. It is possible to have several of these loops. *'logarithmic_step'* is a similar feature for geometric series. The input of the output time is to be finished with the keyword *'end_of_simulation '*.

Driving File

```
...
#
# Time input data
# ==========
# Finish input of output times (in seconds) with 'end_of_simulation'
# 'regularly-spaced' outputs can be set with 'linear_step'
# or 'logarithmic_step' and then specifying the increment
# and end value
00.25
01.00
linear_step 00.50 10.00
linear_step 01.00 25.00
end_of_simulation
# Time-step?
# Options: (real) automatic [0<factor_1<=1] [0<=factor_2] [max.] [min.]
# (Fix time steps: just input the value)
automatic
# Number of iterations for initialisation?
25#
...
```

Then the time step for the phase-field solver is to be specified. It is extremely advisable to use automatic time-stepping apart from some pathological cases: this should therefore be used by default. If you nevertheless want to use constant time-step, here are a few guidelines to follow: the minimum value for the time step consistent with the diffusion parameters is displayed on screen during initialisation (after reading all the input), MICRESS will not perform simulation with too high a time-step. As a general rule, the user can set the time-step between one half and one third of this value as a (relatively) error-free guess. Please note that when 'automatic mobility' is used, the interfacial mobilities and the time-step are dependant (see paragraph 5.10 Phase interaction data).

MICRESS on-screen output

```
...
# Beginning of initialization
# ================
[...]
# Routine init calls routine initTwidth
# tWidth_max( 1: 1) = 0.1187500 s
# tWidth_max( 1: 2) = 0.2375000 s
# tWidth_max( 2: 2) = 0.7916666E-01 s
# Maximal value for tWidth = 0.7916666E-01 s for Phase-field
# Maximal value for tWidth = 9.3571907E-05 s for Conc-field
[...]
...
```

Before starting the simulation MICRESS can perform several preliminary iterations to generate a smooth interface (which is originally input with a sharp interface, and is therefore out of equilibrium in the phase-field description) after which the simulation time is set to zero.

5.9 Phase data.

First input the number of phases, then, for each phase, whether recrystallisation should be simulated, the type of anisotropy for each solid phase have to be specified, and can be set to "*isotropic*", "*anisotropic*" or "*faceted*", and the type of crystal symmetry. The grains of each phase can be sorted in a user-defined number of 'categories': this can speed simulations, as some operations in MICRESS are quadratic with respect to the number of grains (or categories).

Finally the user can set how the orientation of the grains will be defined: as a 2D or 3D Euler angle, rotation angles with respect to the axes, or Miller indices.

Driving File

```
                                    …
#
# Phase data
# ========
# Number of distinct solid phases?
2
#
# Data for phase 1:
# -------------------
# Simulation of recrystallisation in phase 1 ?
# Options:  recrystall  no_recrystall
no_recrystall
# Is phase 1 anisotrop?
# Options:  isotropic  anisotropic  faceted
isotropic
# Should grains of phase 1 be reduced to categories?
# Optionen:  categorize no_categorize
no_categorize
[…]
#
# Orientation
# -------------
# How shall grain orientations be defined?
# Options:   angle_2d
#          euler_zxz
#          angle_axis
#          miller_indices
angle_2d
```

5.10 Grain input data.

Information concerning the microstructure at the beginning of the simulation has to be entered. The first parameter to specify is the type of positioning for the grain present at the beginning, which can either be '*deterministic'* '*random'*, or even read from a text file ('*from_file*'). Then the number of grains which are to be present at the beginning is asked. The next inputs strongly depend on the type of positioning chosen.

Driving File

```
                                    …
#
#
# Grain input
# ========
# Type of grain positioning ?
# Options: deterministic  random  from_file
deterministic
[…]
                                    …
```

5.10.1 Coordinates.

The reference point is the bottom left-hand corner (all point within the simulation domain having positive x , y and z –coordinate).

5.10.2 Deterministic grain positioning.

First the type of grain geometry is asked: it can be *'round'* (i.e.: spherical), *'rectangular'* or *'elliptic'*: please note that this only applies to the 'set' shape, which can be modified by the Voronoi construction (see hereafter). The coordinates, radius (or length of sides for *'rectangular'* or axis for *'elliptic'*) should be specified.

Then the type of description to be used for the curvature has to be specified: it can either be '*stabilisation*' or '*analytical_curvature*', the latter being mostly suitable for grains whose radii are smaller than (or of the order of) the grid-spacing, the former takes affects only with grains which are smaller than a grid-cell.

By default, MICRESS uses a Voronoi construction for regions where grains overlap, this behaviour can be changed with the '*voronoi* / *no_voronoi*' flag which causes grains to set 'over' the other ones. The phase of each grain is also asked. If the grain's phase is not isotropic, its orientation has to be set. If the phase is one for which recrystallisation is simulated, the user is also prompted for a stored energy (in $J.cm^{-3}$).

Driving File

```
                                   ...
#
# Grain input
# =======
# Type of grain positioning ?
# Options: deterministic random from_file
deterministic
# Number of grains at the beginning?
9
# Geometry?
# Options: round rectangular elliptic
round
# x,z coordinates [micrometers], grain number 1?
102.480003
41.9399986
# Grain radius? [micrometers]
46.7200012
# Shall grain 1 be stabilized or shall
# an analytical curvature description be applied?
# Options: stabilisation analytical_curvature
stabilisation
# Voronoi criterion will be applied
# Options: voronoi no_voronoi
voronoi
# Phase number? (integer)
1
[...]
```

5.10.3 Random grain positioning.

The user has to specify how many 'types of grains' are to be defined and how many grains of each type are to be set.

Then these types have to be defined setting the 'geometry', minimum and maximum values for coordinates, radii (in micrometers), what kind of treatment of the curvature should be applied, flag for the Voronoi construction, phase, and, if applicable, and stored energy. Afterwards, if the considered phase is anisotropic, the orientation of the grains has to be defined: it can either be completely random, fixed, or within a defined range. Finally if the grains' phase is to be categorised, the number of categories into which the grains have to be sorted can be specified.

Driving File

```
                                        ...
#
# Grain input
# ========
# Type of grain positioning ?
# Options: deterministic random from_file
random
# Integer for randomization?
13
# Number of different types of grains?
2
# Number of grains of type  1?
100
# Number of grains of type  2?
30
# Input for grain type 1
# ----------------------
# Geometry of grain type 1
# Options: round rectangular elliptic
round
# Minimal value of x-coordinates? [micrometers]
0.0000000E+00
# Maximal value of x-coordinates? [micrometers]
8.000000
# Minimal value of z-coordinates? [micrometers]
4.000000
# Maximal value of z-coordinates? [micrometers]
8.000000
# Minimum grain radius? [micrometers]
1.000000
# Maximum grain radius? [micrometers]
1.000000
# Shall grain type 1 be stabilized or shall
# an analytical curvature description be applied?
# Options: stabilisation analytical_curvature
stabilisation
# Voronoi criterion for grains of type 1 will be applied
# Options: voronoi no_voronoi
voronoi
# Phase number for grain type       1? (int)
1
# Minimum of recrystallisation energie? [J/cm**3]
0.0000000E+00
# Maximum of recrystallisation energie? [J/cm**3]
0.0000000E+00
# Determination of grain orientations?
# options: random fix range
range
# Minimal value of rotation angle ? [Degree]
0.0000000E+00
# Maximal value of rotation angle ? [Degree]
10.00000
# Minimal distance between grains (real) [microns]?
0.5000000
[...]
                                        ...
```

5.10.4 Read initial microstructure from a file.

The starting grain structure can also be read from an ASCII file which will be interpreted as a map of domain displaying the grains' number (similarly to the *'korn'* output) or marking the interfaces (similar to the 'phase' output when only one phase is present).

Driving File

```
                        ...
# Grain input
# ===========
# Type of grain positioning ?
# Options:  deterministic   random   from_file
from_file
# File for grain properties
Microstructure.txt
# Read grain properties from a file?
# Options:    input      from_file
input
# Number of grains at the beginning?
49
# Treatment of data?
# (none, 1D, flip (bottom<->top), or transpose)?
transpose
# AnzX for initial microstructure?
500
# AnzZ for initial microstructure?
400
# Phase number?   (integer)
1
                        ...
```

The user has to supply the name of the file, the dimensions of the map being read (which doesn't have to be the same as the simulation's), the number of grains actually read in, the type transformation to be applied to the data set (transposed and / or flipped, 'phase to grain' or none), and the number of points it contains (which can be different from the simulation domain). All geometric information concerning the grains is obviously already supplied, so the user only has to specify the other relevant grain properties: phase, stored energy, orientation, etc. Please see the corresponding section in the "Fully Answered Questions" (paragraph 10.3), and the "grain growth" standard examples can also be looked-up as a reference.

5.11 Nucleation parameters.

Afterwards nucleation parameters can be defined, the first of them being a flag for nucleation, which can be set to *'no_nucleation'* to disable further nucleation. If so, the following inputs are skipped (as they are not relevant).

The first of these parameters is a flag causing an additional output to be written out when nuclei are set (or a phase disappears). The next input is the number of type of seeds

For each of these types of seeds, their 'position', namely '*bulk*', '*region*', '*interface*', '*junction*' (higher-order junction), or '*quadruple*' has to be specified. Unless the additional keyword '*restrictive*' is specified, triple-junctions are considered to be also part of the binary interfaces, and the interfaces are also treated as pertaining to the bulk. If a nucleation region is requested the user should then define it by its coordinates (in micrometers).

Then the phase of the seeds and the matrix phase for nucleation have to be specified. If the seeds are to be set in the bulk or in a region, the user also has to specify which nucleation model has to be used: '*seed_undercooling*' (i.e.: a new grain is set as soon as a critical undercooling is reached) or '*seed_density*' which is more suitable when a heterogeneous nucleation situation is considered. The former is used by default for nucleation at the interfaces and higher-order junctions. For the sake of brevity, only the '*seed_undercooling*' case will be described here.

Driving File

```
                                        ...
# Data for further nucleation
# ===================
# Enable further nucleation?
# Options:    nucleation      no_nucleation
nucleation
# Additional output for nucleation?
# Options:    out_nucleation    no_out_nucleation
no_out_nucleation
# Data for further nucleation
# ----------------------------
# Number of types of seeds?
1
# Input for seed type 1:
# ------------------------
# Type of 'position' of the seeds?
# Options: bulk region interface triple quadruple [restrictive]
junctions
# Phase of new grains?
2
# Reference phase?
1
# maximum number of new nuclei 1?
250
# Grain radius [micrometers]?
0.0000
# Choice of growth mode:
# Options:   stabilisation analytical_curvature
stabilisation
# min. undercooling [K] (>0)?
50.000
# Shield effect:
# Shield time [s] ?
20.000
# Shield distance [micrometers]?
2.5000
# Nucleation range
# min. nucleation temperature for seed type 1
1000.0
# max. nucleation temperature for seed type 1
1200.0
# Time between checks for nucleation? [s]
1E-1
# Max. number of simultaneous nucleations?
# ------------------------------------------------
# (set to 0 for automatic)
0
# Shall metastable small seeds be killed?
# ----------------------------------------
# Options:    kill_metastable      no_kill_metastable
no_kill_metastable
#
                                        ...
```

In the case of nucleation at an interface, a substrate phase can be specified to take into account the curvature undercooling: this option can be disabled by specifying the reference phase as a substrate phase.

Then the maximum number of these seeds has to be specified (please note that this total might not be reached if the conditions do not allow it). Their radius can be set: it should be chosen carefully as the nuclei might be off equilibrium in the phase-field description, this value should not be so low to let them redissolve. An indicative value (based on the of critical nucleation radius for homogeneous nucleation) is given on-screen at the beginning of the simulation (when Thermo-Calc™ coupling is not activated). A workaround is to set the 'growth mode' of the seeds to '*stabilisation*', which will free then from the curvature term of the phase-field equation until they reach a sufficient size.

MICRESS on-screen output

```
                                   …
# Beginning of initialization
# ================
                                   …
# Critical grain radius:
# of Phase 2 in Phase 1 = 2.50000 / dT_unt [micrometers]
                                   …
```

Then the value of the constitutional undercooling triggering nucleation (in Kelvin, counted as positive), or the minimum stored energy (in J.cm^{-3}), if recrystallisation is taken into account for any phase has to be specified. The 'shield effect' data are to be set: they include the 'shield time' (latency time after new nuclei are sets, during which nucleation is temporarily disabled around them), and shield distance (radius of the zone centred on the nuclei in which nucleation is disabled, in µm). These parameters can have a quite a dramatic influence on the resulting microstructure.

If applicable the way of setting the seeds orientation has to be specified: it can either be '*random*', '*fix*', '*range*', or '*parent_relation*': this should hopefully be self-explanatory. If the grains' phase is to be categorised, the number of distinct 'categories' (orientations) into which the grains have to be sorted can be specified

Minimum and maximum nucleation temperatures for each seed type to be nucleated have to be specified afterwards.

Then the (simulation) time (in seconds) between checks for nucleation has to be input, the main influence of this parameter is to speed-up the calculation: it can therefore be left to 0 (automatic) as a first try.

Some noise can be added to the calculation of the driving force for nucleation (flag '*nucleation_noise*' '*no_nucleation_noise*'), if set, the coefficient for the noise level and a seed for the random number generator will be asked. The noise is applied as $\Delta G \leftarrow \left(1 + k \times \left(random - \frac{1}{2}\right)\right)\Delta G$ (where $0 \le random \le 1$ is the output of the random number generator and ΔG the driving force for nucleation: constitutional undercooling or stored energy).

In some cases the user might wish to limit the number of nucleations events per call to the nucleation routine: this can be done afterwards.

In some cases, 'stabilised' nuclei can reach a metastable state at which they do not grow any more (as they are meant to), but nevertheless do not vanish because the weighting of the curvature term in the phase-field equation slows their disappearance to a standstill. It is possible to terminate the nuclei that have not grown enough between two consecutive call to the nucleation routine (hence the importance of this parameter in this case), by enabling *'kill_metastable'*, this flag can also be set to *'no_kill_metastable'*.

5.12 Phase interaction data.

Physical data for the interaction of each phase with the others are entered afterwards. Each of this can be disabled by setting the parameter to *'no_'*.

Solid-state inter-action between grains of the same phase can be simulated when the interaction of one phase with itself is enabled.

The surface energy and kinetic coefficient are to be set. The mobility and surface energy can be input as constant values or treated as temperature-dependant parameters, in which case a text file describing this dependency has to be specified. These files should consist of two columns: the first being the temperature and the second the value of the corresponding mobility or surface energy at this temperature. A linear interpolation will be performed between the values supplied by the user. Please note that the check for the compliance of the mobility, surface energy and constant time-step with the stability criteria has been disabled in this case.

Driving File

```
                                        …
# Phase interaction data
# ==============
#
# Data for phase interaction 0 / 1:
# ---------------------------------
# Simulation of interaction between phase 0 and 1 ?
# Options:  phase_interaction  no_phase_interaction
#           [standard|particle_pinning|solute_drag]
no_phase_interaction
[…]
# Data for phase interaction 1 / 1:
# ---------------------------------
# Simulation of interaction between phase 1 and 1 ?
# Options:  phase_interaction  no_phase_interaction
#           [standard|particle_pinning|solute_drag]
phase_interaction
# Type of surface energy definition between phases 1 and 1?
# Options: constant temp_dependent
constant
# Surface energy between phases 1 and 1? [J/cm**2]
1.00000E-05
# Type of mobility definition between phases 1 and 1?
# Options: constant temp_dependent sd_kth dg_dependent
constant
# Kinetic coefficient mu between phases 1 and 1? [cm**4/(Js)]
1.00000E-05
#
                                        …
```

Another option for the mobility is the solute-drag model from KTH where an effective mobility dependant on the driving force is used, see article [14] of the references.

An additional flag can also be set to specify the interaction model to be used: standard (i.e.: standard phase-field equation), particle pinning, or solute drag. These two models are described in the articles [6] and [7] of the references, they are based on a two-steps hysteresis description of the mobility, respectively as a function of interface velocity (for solute drag) or driving force (for particle pinning).

The solute drag effect is considered to be dependent on the mobility of the interface. To model this behaviour three parameters are necessary: the reduction of the mobility (drag factor, coefficient (<1) correcting the mobility at low velocities), the critical velocity setting the limit for solute drag, and a transition range within which the mobility changes linearly between the mobility values with and without solute drag.

Particle pinning is modelled as a dependence of the mobility on the driving force calculated from the local curvature. Two parameters are needed: the minimal mobility and the critical curvature.

A few more parameters have to be specified for interactions between different phases: first the 'delta G' options, which control respectively the averaging along the normal to the interface, cutting off the driving force, and the 'smoothing'. They are to be input in one line with keywords, what is not specified will be set to default, if everything should be set to default, use 'default' as a place holder. For information, the effective values are mirrored right after the input.

Driving File

```
                                                    ...
# Phase interaction data
# ===============
#
# Data for phase interaction 0 / 1:
# --------------------------------
# Simulation of interaction between phase 0 and 1 ?
# Options:  phase_interaction  no_phase_interaction
#           [standard|particle_pinning|solute_drag]
phase_interaction
# 'DeltaG' options:  default
#            avg ... []  max ... [J/cm**3]  smooth ... [degrees]
avg 1  max 20
# I.e.:  avg +1.00  smooth +45.0  max +2.00000E+01
# Type of surface energy definition between phases LIQUID and 1?
# Options:  constant  temp_dependent
constant
# Surface energy between phases LIQUID and 1? [J/cm**2]
2.04000E-05
# Type of mobility definition between phases LIQUID and 1?
# Options:  constant  temp_dependent  sd_kth  dg_dependent
constant
# Kinetic coefficient mu between phases LIQUID and 1? [cm**4/(Js)]
4.00000E-03
# Is interaction isotropic?
# Options:  isotropic  anisotropic
anisotropic
# static anisotropy coefficient? (< 1.) (changed!!!)
0.3000000
# kinetic anisotropy coefficient? (< 1.)
0.3000000
#
```

The averaging factor, with the keyword 'avg': this is a value between 0 (no averaging) and 1 (average to the infinite), with 0.5 for averaging over the interface's length. This feature is only activated if the "averaging of the driving force along the normal to the interface" has been enabled, and is meant to help stabilising the interface.

Compatibility note: this input has the same purpose as the previous averaging length, but a different definition: $\text{averaging factor} \approx \frac{\text{averaging length}}{\text{interface thickness} + \text{averaging length}}$

The directional averaging can be specified via the keyword 'smooth': this enables averaging not only along the normal itself, but also with some deviation, which helps minimising the effects of the grid anisotropy. Please note that directional averaging is enabled only when averaging (along the normal to the interface) is. It can also be disabled by setting it to a negative value.

The maximal driving force allowed (value above which the driving force will be cut-off), can be specified with the keyword ‘max’: this is useful to shrug off some temporary problems during transients or fluctuations. Just omit the input to disable (this is the default!), as a negative value will 'blank' 'ΔG', i.e.: only take into account the curvature part of the driving force...

The description of the interaction between an 'anisotropic' phase and an 'isotropic' one also includes a flag for the anisotropy, and if this is switched on, the static and kinetic anisotropy coefficients have to be specified.

5.13 Diffusion data.

The diffusion parameters have to be specified. First the number of dissolved constituents is set.

Afterwards the user has to choose whether the concentrations will be set in atom or weight percents.

For each component and phase the diffusion flag should be set: the available options are '*diff*', '*no_diff*', '*infinite*', '*stoichio*', '*database_blobal*', *database_local*', and '*multi*'. The meaning of the first four should be self-explanatory. Setting '*database*' means that the diffusion coefficients will be calculated by Thermo-Calc™ (via its TQ interface): this is only possible when the ‘GES-file’ used also contains mobility data. '*multi*' means that the complete Fick-Onsager equations will be solved, including the so-called ‘off-diagonal terms’ of the diffusion matrix. It is possible to qualify '*multi*' and use ‘global’ or ‘local’ diffusion coefficients from a database (‘local’ means that they are linearly interpolated inside a phase to reflect the influence of composition), user-defined or simply ignored. If '*diff*' has been selected, the pre-exponential factor and its activation energy (which can be set to 0 for no temperature

Driving File

```
                                        ...
# Concentration data
# =============
# Number of dissolved constituents?  (int)
2
# Type of concentration?
# Options:    atom_percent   (at%)
#             weight_percent  (wt%)
weight_percent
#
# Options: diff   no_diff   infinite   multi
#          database_global   database_local
#          [+b] for grain-boundary diffusion
# ('multi' can be followed by a string of "n", "d", "g", or "l",
#  to describe each contribution: respectively no diffusion,
#  user-defined diffusion coefficient, and 'global' or 'local'
#  value from database, the default is global values from
database).
# How shall diffusion of component 1 in phase 0 be solved?
no_diff
# How shall diffusion of component 1 in phase 1 be solved?
diff
# Diff.-coefficient:
# Prefactor? (real) [cm**2/s]
0.23400
# Activation energy? (real) [J/mol]
1.47700E+05
                                        ...
```

dependence) of the diffusion coefficient have to be specified. In the case of a stoichiometric phase a diffusion coefficient can nevertheless be input for numerical reason (it can be set 0 if not needed).

It is also possible to request enhanced diffusion at the grain boundaries with “+b” followed by a string consisting of “b” and “n” (to respectively en- or disable this feature for the corresponding grain boundaries). When this feature is used, the user is prompted for the correction of the activation energy at the interface, and the physical width of the interface.

5.14 Phase diagram data.

The first information required is a list of the stoichiometric components.

The user then has to specify whether Thermo-Calc™ coupling is to be used (as opposed to the input of a linearised phase diagram), which can be respectively set with 'database' or 'no_database'.

The following depends heavily on this choice and has therefore been split in two sub-sections.

Driving File

```
...
#
# Phase diagram - input data
# ==================
#
# List of phases and components which are stoichiometric:
#  phase and component(s) numbers
# End with 'no_more_stoichio' or 'no_stoichio'
no_stoichio
#
# Is a thermodynamic database to be used?
# Options: database   no_database
no_database
#
...
```

5.14.1 Linearised phase diagram.

If the Thermo-Calc™ coupling (via its TQ interface) is switched off (or a phase interaction is set to '*linear*'), the values relative to the linearised phase diagram have to be set.

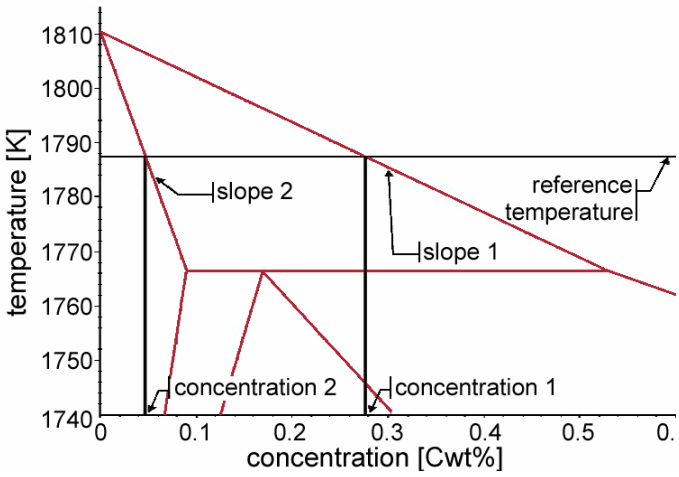
They have to be input by pair-wise relation: data related to the equilibrium of phase 0 and 1 (i.e.: phase 1 and liquid), 0 and 2, and so on. When all relations concerning the liquid phase have been described, those describing solid phases' equilibrium have to be input: 1 and 2, and others if needed. (The equilibrium between phases which are not interacting doesn't need to be described).

They include the reference temperature (at which the linearization was performed), the entropy of transformation, the concentration of each components in the considered phases, and the corresponding slopes.

For multi-component systems the descriptions becomes lengthier, but the formalism is the same.

Driving File

```
...
# Is a thermodynamic database to be used?
# Options: database   no_database
no_database
# Input of the phase diagram of phase 1  and phase 2:
# ------------------------------------------------------------
# Temperature of reference point? [K]
1149.9000
# Entropy of fusion between phase 1  and 2  ? [J/(cm**3 K)]
0.14900
# Input of the concentrations at reference point
# Concentration of component 1  in phase 1 ? [wt%]
0.32000E-02
# dissolved concentration in phase 2 ? [wt%]
0.15811E-03
# Concentration of component 2  in phase 1 ? [wt%]
0.17399
# dissolved concentration in phase 2 ? [wt%]
0.96288E-01
# Input of the slopes at reference point
# Slope m_iPh = dT/dC_iPh relative to component 1  ? [K/wt%]
-386.5673523
# Slope m_jPh = dT/dC_jPh relative to component 1  ? [K/wt%]
-8036.549805
# Slope m_iPh = dT/dC_iPh relative to component 2  ? [K/wt%]
-39.82677078
# Slope m_jPh = dT/dC_jPh relative to component 2  ? [K/wt%]
-73.34864807
```



5.14.2 Thermo-Calc™ coupling via its TQ interface.

To use Thermo-Calc™ coupling, a 'GES-file' is needed, this is the first input to be supplied.

The frequency for complete relinearization has to be set.

Then, in a similar way to what is done without coupling, the phase interactions are gone through: each equilibrium can be described by the TQ interface of Thermo-Calc™ or with a linearised phase diagram (in which case the input is similar to 5.10.1): this is set with 'TC' or '*linear*'.

If Thermo-Calc™ is used, a maximum temperature deviation for re-linearization has to be specified. Setting a high value speeds up the calculation by limiting the number of calls to the TQ library (at the expense of precision). An input of '-1' can be used to switch off the relinearisation triggered by temperature deviation.

The Thermo-Calc™ index of each (MICRESS) component and phase is then to be set. MICRESS displays at run-time the list of components and phases available in the selected 'GES-file'.

Driving File

```
...
# Is a thermodynamic database to be used?
# Options: database   no_database
database
# Name of Thermo-Calc *.GES5 file without extension?
GES_Files/Al_Cu
# Frequency for complete relinearization [s] =
100.
# Input of the phase diagram of phase 0  and phase 1:
# ------------------------------------------------------
# Which phase diagram is to be used?
# Options: database  linear
database
# Maximal allowed local temperature deviation [K]
-1.
# The database contains the following components:
#   AL
#   CU
# Specify relation between component indices Micress -> TC!
# The main component has in MICRESS the index 0
# Thermo-Calc index of (MICRESS) component 0?
1
# Thermo-Calc index of (MICRESS) component 1?
2
# The database contains 2  phases:
#   LIQUID
#   FCC_A1
# Specify relation between phase indices Micress -> TC!
# The matrix phase has in MICRESS the index 0
# Thermo-Calc index of the (MICRESS) phase 0?
1
# Thermo-Calc index of the (MICRESS) phase 1?
2
# Molar volume of (MICRESS) phase 0? [cm**3/mol]
10.
# Molar volume of (MICRESS) phase 1? [cm**3/mol]
10.
# Temperature at which the initial equilibrium
# will be calculated? [K]
914.
```

Afterwards the user is prompted for molar volume of each phase.

The final input of this section is the temperature for the initialisation by Thermo-Calc™ of the interactions of phases present at the beginning of the simulation.

It is possible to tweak the size of TQ's workspace by adding an optional line starting with the keyword 'wokspace_size' followed by the requested size in kilo-bytes after the specification of the 'GES-file'. The following input remaining unchanged.

Driving File

```
...
# Is a thermodynamic database to be used?
# Options: database   no_database
database
# Name of Thermo-Calc *.GES5 file without extension?
GES_Files /Fe_C_Mn_Si_P
# TQ's 'workspace' size? (in kilo-bytes)
workspace_size 100000
...
```

5.15 Initial concentrations.

Input of the initial concentration: three possibilities are available: explicitly setting the concentration for each phase (with '*input*'), specifying only the initial concentration of one phase, and using the equilibrium concentrations for the other phases is also possible (with '*equilibrium*'). Finally, similarly to what is done for the initial grain structure, the initial concentration field can be read from a file (with '*from_file*').

Driving File

```
                              ...
#
# Initial concentrations
# ======================
# How shall initial concentrations be set?
# Options:  input  equilibrium  from_file   [phase number]
input
# Initial concentration of component 1 in phase 0? [wt%]
0.E+0
# Initial concentration of component 1 in phase 1? [wt%]
3.299999982E-3
# Initial concentration of component 1 in phase 2? [wt%]
1.999999955E-2
# Initial concentration of component 2 in phase 0? [wt%]
0.E+0
# Initial concentration of component 2 in phase 1? [wt%]
0.173999995
# Initial concentration of component 2 in phase 2? [wt%]
0.400000006
#
                              ...
```

If '*input*' is used, the initial concentrations of each constituent in each phase have to be selected, even for phases which might not be initially present (in this case, this value is of little significance).

If '*equilibrium*' is chosen: the concentration only have to be set for a reference phase, which is by default the liquid, but can be any other one present at the beginning (its index should then be specified in the same line).

5.16 Elastic material data

This only applies *'stress'* and *'stress_coupled'* simulations. The first input is the phase number of a matrix phase. The strain and the calculation of the Eigenstrains will be referenced to this phase. Then for each phase its molar volume and three tensor coefficients of Hooks matrix in Voigt-notation C_{11}, C_{12}, C_{44} are the necessary input. With these parameters isotropic and cubic lattice symmetries can be represented.

Driving File

```
                              ...
# Input of materal data for elastic calculation
# =============================================
#
#
# Phase number of the matrix phase (int)
1
# Abstraction of the 3D continuum
#   Options:  plane_stress  plane_strain
plane_stress
#
#
# phase 0
# -------
# molar volume [cm**3], phase 0
7.18240023
# Elastic components (Voigt-notation)
# C11 [MPa] ( >0 )      , phase 0
23300.
# C12 [MPa] ( >0, <C11 ), phase 0
13300.
# C44 [MPa] ( >0 )      , phase 0
11600
                              ...
```

5.17 Temperature data.

In the case of temperature coupling, the phase equilibrium can be described only with the equilibrium temperature and the entropy of fusion.

The other inputs are the heat conductivity (λ), heat capacity (ρC_p) and latent heat for each phase.

The two former can be input as constant values or treated as temperature-dependant parameters, in which case a text file describing this dependency has to be specified. These files should consist of two columns: the first being the temperature, and the second the value of the corresponding material property at this temperature. A linear interpolation will be performed between the values supplied by the user.

Driving File

```
...
#
#
# Phase diagram - input data
# ==================
#
# A description of each pairwise thermodynamic
# interaction has to be specified.
#
# Equilibrium temperature (real) [K] between 0  and 1
1000.000
# Entropy of fusion between phase LIQUID  and 1 ? (real) [J/(cm**3 K)]
0.5000000
#
# Temperature Data
# ============
# Type of thermal conductivity definition for phase 0 ?
# Options:    constant    temp_dependent
constant
# Thermal conductivity of phase 0 ?  (real) [W/cm/K]
0.5000000
# Type of thermal conductivity definition for phase 1 ?
# Options:    constant    temp_dependent
constant
# Thermal conductivity of phase 1 ?  (real) [W/cm/K]
0.5000000
# Type of specific heat capacity definition for phase 0 ?
# Options:    constant    temp_dependent
constant
# Specific heat capacity of phase 0 ?   (real) [J/cm**3/K]
1.000000
# Type of specific heat capacity definition for phase 1 ?
# Options:    constant    temp_dependent
constant
# Specific heat capacity of phase 1 ?   (real) [J/cm**3/K]
1.000000
# latent heat for phase interaction 0 / 1?      (real)  [J/cm**3]
10.00000
#
...
```

5.18 Latent heat parameters.

In this section, specific input data for the release of latent heat are defined, which can be simulated (or not) by specifying '*lat_heat*' to or '*no_lat_heat*'. Then, the enthalpy of each phase (including the liquid), as well as its specific thermal capacity has to be specified.

Driving File

```
                                    ...
#
# Parameters for latent heat
# ========================
# Simulate release of latent heat?
# Options:   lat_heat   lat_heat_3d [matrix phase]   no_lat_heat
lat_heat
# Enthalpy of phase 0? ([J/cm^3])
0.E+0
# Specific heat capacity (Cp) of phase 0? ([J/(cm^3*K)])
2.43
# Enthalpy of phase 1? ([J/cm^3])
-1231.
# Specific heat capacity (Cp) of phase 1? ([J/(cm^3*K)])
2.43
# Enthalpy of phase 2? ([J/cm^3])
-1231.
# Specific heat capacity (Cp) of phase 2? ([J/(cm^3*K)])
2.43
#
                                    ...
```

As the time to reach thermal equilibrium is considered negligible compared to the characteristic times for diffusion the release of latent heat is treated as a 'global warming': the temperature of the whole simulation domain being raised uniformly.

If the release of latent heat is enabled, the specification of the variation of temperature is made via the input of a heat flux, and the 'Moving frame' feature is automatically disabled (see hereafter).

5.19 Boundary conditions.

Some other conditions have to be set.

The first of those are related to temperature: the initial temperature: the type of variation (which should be left to '*linear*'), the number of transition points, as the temperature conditions can be set by intervals. Then for each of these transition points (including t=0), the time (except, of course for t=0), the temperature at the bottom and the temperature gradient (in the z direction). The temperature and temperature gradient are linearly interpolated between these transition points.

Driving File

```
                                    ...
#
# Boundary conditions
# ==============
# Type of temperature trend?
# Options: linear     linear_from_file     sinus
linear
# Number of connecting points?    (integer)
2
# Initial temperature at the bottom?  (real)  [K]
1150.
# Temperature gradient in z-direction?  [K/cm]
0.E+0
# 1  Connecting point, time  t [sec]?
2.5
# 1  Connecting point, temperature
1125.
# 1  connecting point, temp. gradient in z-direction [K/cm]
5.
# 2  Connecting point, time  t [sec]?
7.5
# 2  Connecting point, temperature
1000.
# 2  connecting point, temp. gradient in z-direction [K/cm]
25.
                                    ...
```

It is also possible to read this information from a file consisting of three columns storing respectively the time in seconds, the temperature at the bottom in Kelvin, and the gradient in Kelvin per centimeter.

Driving File

```
...
#
# Boundary conditions
# ==============
# Type of temperature trend?
# Options: linear      sinus
linear
# Number of connecting points?    (integer)
0
# Initial temperature at the bottom?  (real)  [K]
1155.
# Temperature gradient in z-direction?  [K/cm]
0.E+0
# Cooling rate? [K/s]
-25.
...
```

Finally, is also possible to describe the temperature evolution by a single cooling rate and temperature gradient, in which case the number of transition points should be set to 0

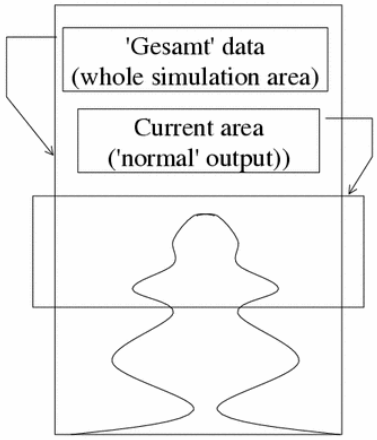
If the release of latent heat is enabled, a heat flux (in Js/cm^3) has to be specified instead of a temperature (or cooling rate).

Then the 'moving frame' options have to be set: this feature is very useful for simulations related to directional solidification, as it allows the actual solving to be done on only part of the simulation domain (therefore reducing CPU time). If the flag *'moving_frame'* is not set to *'no_moving_frame'*, the user is prompted for the criteria causing points to be shifted out of the simulation domain: this can be 'temperature' or 'distance'. In the case of 'temperature', it is linked to a temperature below which the points have to be shifted out of the simulation domain. For 'distance', it is the minimal distance between the solid phases and the top of the simulation domain. In both cases, the corresponding value has to be input afterwards.

Driving File

```
...
# Moving-frame system in z-direction?
# Options:     moving_frame     no_moving_frame
moving_frame
# Should the distance or the bottom temperature be
# used as criterion for moving frame?
# Options:  distance  temperature
distance
# At which distance from the upper boundary the frame should
# be moved?  (real)  [micrometers]
200.0000
# Store data shifted out of moving-frame system?
# Options:     out_moving_frame     no_out_moving_frame
no_out_moving_frame
...
```

Saving the data related to these points is directed by the *'out_moving_frame'* flag: creating (or not) 'Gesamt' (global) data for all selected outputs: these files have 'G' appended to their 'root name' (i.e.: *'Simulation.phas'* and *'SimulationG.phas'* under Unix).



The assumptions made to simulate the release of latent heat are deemed to be incompatible with the use of the moving frame feature, it is therefore disabled in this case.

The boundary conditions should be set for phase-field, concentration, temperature and displacement field depending on the type of coupling which had been defined in the beginning. The boundary conditions can be insulation, periodic (wrap-around), symmetric (the domain boundary being treated as a local symmetry plane), gradient or fixed (a fixed value is set for the corresponding field at the corresponding interface) in the case of phase field, temperature and concentration.

Driving File

```
...
# Boundary conditions for phase field in each direction
# Options: i(insulation) s(symmetric) p(periodic/wrap-around) g(gradient) f(fixed)
# Sequence: E W (N S, if 3D) B T borders
pppp
#
# Boundary conditions for concentration field in each direction
# Options: i(insulation) s(symmetric) p(periodic/wrap-around) g(gradient) f(fixed)
# Sequence: E W (N S, if 3D) B T borders
pppp
# Unit-cell model symmetric with respect to the x/y diagonal plane?
# Options:   unit_cell_symm   no_unit_cell_symm
no_unit_cell_symm
...
```

Additional boundary conditions are required in case of stress coupling, the available options are '*constant_volume*' (zero displacement of all boundaries), '*free_expansion*' (bottom left corner fixed, free expansion in all directions) and '*parallel_expansion*' (bottom left corner fixed, free expansion along main axes). Furthermore external stress and strain acting on the simulation domain can be defined. The boundary conditions are '*fix_isostatic_pressure*', '*fix_isostatic_strain',* '*fix_normal_pressure'* and '*fix_normal_strain',* accordingly. For the *'isostatic'* cases either the normal pressure at the domain boundaries or the normal displacement are fixed. The values should be specified in a second line (real numbers, units are [MPa] or [%], respectively. The *'normal'* variants allow the definition of normal displacement or normal stress in each direction separately. In all cases the domain will expand according to the option '*parallel_expansion*'.

Driving File

```
...
# Boundary condition for elastic stress calculation
# Options: constant_volume  normal_expansion  free_expansion
#          fix_isostatic_pressure  fix_normal_pressure
#          fix_isostatic_strain    fix_normal_strain
fix_isostatic_strain
# Isostatic strain?    +/- (real) [%]
1
...
```

An attempt can also be made to try to keep some kind of symmetry with respect to the x/y diagonal: '*unit_cell_symm*' and '*no_unit_cell_symm*' are the available options.

Then, the maximum number of concentration solving per phase-field iteration has to be entered (in the case of concentration coupling). This input is not required with automatic time-stepping. There is no strong influence on the results or performance. If the value is too small, a warning is issued.

Driving File

```
...
#
# Other numerical parameters
# ==================
# Maximum number of calls of the concentration solver per iteration?
500
# Phase minimum?
9.999999747E-5
# Interface thickness (in cells)?
7.5
#
...
```

Φ_{min} should be specified here, it is a deviation limit for the phase-field parameter below which the cell is not considered to be in the interface any more but in a bulk region (be it liquid or solid).

The interface thickness (in cells) also has to be input here.

In case of stress coupling the convergence criteria for the iterative BiCGstab matrix solver as well as an upper limit (maximum number) of iterations has to be defined. In the input line for the maximum number of iterations a second integer input is possible. The number is set to 20 by default and specifies the maximum number of iterations allowed for achieving a good solution for the quasi-static equilibrium. In most cases default settings are sufficient.

6 Known issues.

6.1 Problems with some Linux distributions.

It is currently not possible to run MICRESS® with some Linux distributions: this is mostly due to problem with the licensing package used in MICRESS (FLEXLM™), here is a comment made on Macrovision's website:

> *"Our experience with Linux leads us to believe that it is not the most infallible operating system that we support. This is likely due to the fact that the operating system can be easily customized - presenting advantages and disadvantages. We have found that each new release of Linux isn't necessarily backwards compatible although each new release does include important enhancements."*

6.2 Restarting simulations.

The 'restart' feature was found not to be entirely accurate in some cases (last digit variations), especially with the coupling to Thermo-Calc™ (via its TQ interface).

6.3 μ(T) and stability criteria.

The check for the compliance of the mobility, surface energy and the constant time-step with the stability criteria has been disabled in the case of a temperature or driving-force dependant mobility. Please use automatic time-stepping in this case.

6.4 Nucleation of liquid.

It is currently not possible to simulate the nucleation of liquid with MICRESS®.

6.5 Image drivers for *Display MICRESS*.

Unfortunately no PNG image driver could be implemented for the PC version of *Display MICRESS*, so instead of 'Transparent PNG' and 'Opaque PNG' the two options available in windows environment are 'Portrait GIF' and 'Landscape GIF'.

7 Post-processing.

MICRESS generates output files for the solutions of different field variables in a binary format. The solutions for the individual time steps are concatenate in one file. For evaluation and visualisation of the output files different post-processing tools are available. A brief description is given in this chapter.

7.1 Available post processing tools.

Display MICRESS:	Visualisation tool for MICRESS result files.
Transfer MICRESS:	Filter for MICRESS result files.
DP MICRESS:	Bundle of the two previous executables. (Note: to increase confusion and generally confound the reader as much as possible, the *DP MICRESS* binaries are nevertheless called *Display MICRESS* and the graphical interface to *Display MICRESS* is called DP_MICRESS).

7.2 Display MICRESS.

Display_MICRESS (*DP_MICRESS*) is a post-processing tool with a wide span of possibilities, ranging from basic display and image output, to advanced features such as zooming, multiple display, build-in four-folded symmetry, animation and 'Virtual EDX'. It can also handle several files simultaneously.
It can read results file in binary (single and double precision, native or not) and ASCII, compressed or not, as well as perform conversions between these formats.

Libraries:

Display MICRESS relies on the following libraries:

- *PGPlot* (www.astro.caltech.edu/~tjp/pgplot) for all graphical operations.
- PNG (www.libpng.orgl) for images output.
- *http://www.zlib.net* is used for compression, by the *PNG* library and for compressing files.
- *GrWin* (http://spdg1.sci.shizuoka.ac.jp/grwinlib/english) is used as a screen driver for *PGPlot* under Windows.

DP_MICRESS, the graphical user interface to *Display MICRESS*:

- is written in *Perl* (www.perl.org).
- uses extensively the *Perl/Tk* module (www.ni-s.u-net.com).
- and is 'packed' as an executable with *PAR* (par.perl.org).

7.2.1 Running *Display MICRESS*.

Display MICRESS can be called from a shell, providing the name of the result file(s) to be displayed (it does not allow switching between files, meaning it shall be restarted to display another file).

It can, for example, be called with:

DP_MICRESS *Test.phas*

(if no argument is provided, a summary of command line-options is returned).

Command-line options:

Main command-line options:

- ⇨ -b: results in binary (single-precision).
- ⇨ -z: read compressed results.
- ⇨ -3,-4,-9: respectively three-, four- or nine-folded symmetry.
- ⇨ -f: read automatic min./max. from the first time-step.
- ⇨ --Min:*value* –Max:*value*: explicitly specify the min. and max. to use.
- ⇨ -m: multiple results: specify the number of result files (integer value following 'm', ex.: -m6).
- ⇨ -p: divide display in panels, row major (two integers separated by 'x' following 'p', ex.: -p2x3).
- ⇨ -q: divide display in panels, column major (ex.: -q2x3).
- ⇨ -g: read run-time instructions from standard input (to allow piping from GUI device).
- ⇨ -t: *Transfer MICRESS* (converts file).
- ⇨ --Animate: animate to the end.
- ⇨ --Help: print a list of all available command-line options.

Default settings:

- ⇨ automatic min./max. from the whole file.
- ⇨ number of panels fits the nb. of solutions.
- ⇨ no graphical user interface (when called from the command line).

Multiple display: this feature is restricted to results files with the same geometry.

Compressed files: the whole files are decompressed to temporary files which are erased when the program is exited, it is therefore preferable to close *Display MICRESS* 'nicely' (i.e.: no interruption), to avoid leaving those files in the working directory.

Non-native files: *Display MICRESS* can handle ‘non-native’ binary results, but the necessary on-the-fly conversion nevertheless takes time: converting the files is often a reasonable option. It is also impossible to display files with different ‘endian-ness’.

Transfer MICRESS:

This tool converts results file to and from the following formats: binary (both single and double precision) and ASCII, compressed or not. The ASCII format is useful to transfer results between platforms. *Transfer MICRESS* can also rename MICRESS® result files using Irix or Windows naming conventions.

It can, for example, be called with:

DP_MICRESS -t *Test_Binary.phas Test_ASCII.phas*

(if no argument apart from '-t' is provided, a summary of command line-options is returned).

Command line:

DP_MICRESS -t [options] [-i]Input_File [[-o]Output_File]
(-i and -o can omitted if file names are specified in that order the output name can be omitted altogether if it is the same as the input).

Available options:

- ⇨ -a: input file in ASCII.
- ⇨ -d: input file in double precision.
- ⇨ -e: input file in binary (single precision).
- ⇨ -y: compressed input file.
- ⇨ -b: output file in binary (single precision).
- ⇨ -f: output file double precision.
- ⇨ -c: output file in ASCII.
- ⇨ -z: compress output file.
- ⇨ -g: input is a geoF file.
- ⇨ -w: transfer whole set of results.
- ⇨ -k: remove output from result file (ex.: -k5 to remove fifth output).
- ⇨ -l: remove sequentially from result file (ex.: -l5 -l7to remove 5th and 7th outputs).
- ⇨ -r: rename set of results from UNIX's naming to Windows' (or vice-versa).

Default:

- ⇨ 'plain' file in binary (not compressed).
- ⇨ output file in ASCII (not compressed).

7.2.2 User interface, typographical conventions.

Display MICRESS has a full-fledged graphical front-end (*DP_MICRESS*) which also acts as a wrapper to *Display_MICRESS* itself. The following describes the use with keyboard shortcuts (via the graphical front-end or not). All operations can be called by 'hot keys', which are not case dependent, e.g. key 'f' and key 'F' are considered to be identical.

Keyboard input:

Apart from the alphanumeric characters, the following keys are also available: ***Escape*** (erases the current input) and ***Tab*** (validate the current input and go the next, if any).

UNIX (and Linux) environment:

The *DP MICRESS* interfaces can be called with '-g' flag: it is possible to call it with only this flag, then an interface to create the command-line is displayed, or with a complete command-line, in which case only the run-time interface is called.

MS Windows:

Double-clicking a *MICRESS* result file will start *Display_MICRESS* with the default settings, otherwise a '*geoF*' file should be double-clicked (to display various files at the same time, or call *Transfer_MICRESS* for example), Please see *'Installing Display_MICRESS under Windows'*.

Typographical conventions:

Keys to be pressed will be printed in ***italics bold***: example ***N*** means press key N (either lower or upper case). The combination of keys D and E (pressing key D then key E) will be represented by ***D+E***.

For an improved readability, the corresponding operation will be printed in *underlined italics*.

Known issues:

When using the graphical user interface, not exiting 'nicely' (i.e.: with the '***EXIT***' button) can lead to complications, please avoid it.

7.2.3 Time-step operations.

These include going to the *next*: ***N***, *previous* ***P***, *last* ***L*** or *first* ***F*** *time-steps*. Hopefully, these operations should be self explanatory.

When several files are displayed simultaneously, these operations can also be applied to a selection of the results only with respectively ***M+N***, ***M+P***, ***M+L*** or ***M+F***.

7.2.4 Scale.

By default minimum and maximum are chosen as the extrema of the whole result file, which implies that the entire file has to be read (which might take some time for very large simulations), unless the '–f' option was set from the command line, and then the automatic min. and max. are set from the local min. and max. of the first time step.

The available options are: *user-defined min. and max.* (***S+M***: a secondary window is opened to let the user modify the min. and max. settings), *user-defined range* (***S+R***: similar to the previous, but min. and max. are set as median value and range), use *local min. and max.*, ***S+D***, which sets the extrema from what is displayed, which can be only part of the result for the current time-step if the zoom is in use, and finally revert to *automatic* (i.e. global) *min. and max.*, ***S+G*** (if the '-f' option was used, the file is then read for the global extrema). ***S+F*** explicitly *force* the *file* to be *re-read* to find out the global extrema.

Note: if several result files are displayed the user will be prompted to select the solutions to which these operations should be applied to. User-defined settings will affect all solutions which are selected simultaneously.

7.2.5 Colour scale.

Various colour scales are available in *Display MICRESS*, the default one being the standard '*Viso heat scale*', but a few others are also available. They can be selected with ***C+1...11***, (for example ***C+1*** sets the (default) '*Viso heat scale*', and ***C+2*** a *black and white* one), ***C+L*** *loops* through the *available colour-scales*. To select 'double-digit' colour scale without graphical user interface, press 0: ***C+0+1+0*** will select the *tenth colour scale*. The tenth and eleventh colour scales (respectively called with ***C+9*** and ***C+010***) are 'adaptive' in the sense that they have ranges of colors and / or transition points whose 'position' in the scale can be reset by the user (according the isoline values).

The *brightness and contrast* can be *fiddled* with by pressing ***C+F***, or *reset* with ***C+R***. This fiddling feature is performed by resetting the brightness with the normalised x-coordinate of the mouse cursor on the active image, and the brightness with y-coordinate's. If a GUI device is used, the user has to click to set the cursor's position after calling this feature.

The *colour-scale* can also be *inverted* with ***C+I***.

The *minimum* and *maximum* of the colour-scale can be *cut-off* (i.e.: respectively replaced with black and white) with ***C+C***. The current colour-scale can also be reset in a *stepwise* fashion with ***C+S***. It is possible to specify the number of step with ***C+U*** (*user-defined*), and to *toggle on and off* the use of this input with ***C+T***. To break some unfortunate patterns when displaying "*grain*" output, it can be

interesting to use a stepwise colour scale, and *randomise* it with ***C+K***. These previous features are unfortunately not available under Windows, due to a 'communication' problem between *PGPlot* and *GrWin*.

7.2.6 Animation.

Display MICRESS supports *animation*, ***A+R*** will display one time step and then automatically switch to the next, looping over the whole file. Unfortunately, it is not possible to interrupt the animation short of killing the program. ***A+E*** starts an *animation to the last output*.

The *animation settings*, display time for each time-step and number of loops can be changed with ***A+S***. The display time might actually have to be extended, to let the program proceed to the next time-step (in the case of large result files or simultaneous display of several solutions).

7.2.7 View.

This category regroups various operations related to the graphical window settings.

Reset number of panels: ***V+P***: this should be self-explanatory. The display can be restricted to a given panel with *Freeze panel*: ***V+F***, this option is only available when a single result file is displayed, all subsequent display will be made in the corresponding panel. This feature is convenient to visualise in the same window specific outputs from a simulation. A secondary window is open, displaying the current panel setting, clicking on one panel selects it, and a second click validates the selection.

Redraw: ***V+R***, which can be useful when the user wants to update the display (for example after changing some display parameter). An *auto-replot* feature is also available with ***V+Q***.

Resize: ***V+S***, makes *Display MICRESS* take into account the possible resizing of the display-window made by the user, and updates the viewport accordingly. An '*auto-resize*' feature can also be switched-on (and off) with ***V+Z***.

Displaying annotations (comments and colour scale) can be set with ***V+A***: four options are available: comments and colour scale (default), colour scale only, annotations only, or none. The *colour scale* can be displayed in a *secondary window* with ***V+C***. Please note that later changes on the scale won't be reflected on this display. The annotations can also be positioned to the left and right of the picture or at the bottom and top, which toggled with ***V+O*** (for *orientation of annotations*), this setting will also be reflected on the colour scale displayed in secondary windows. The *'thickness' of the colour scale* can be increased with ***V+T***, the font size for the comments will also be modified at the same time.

The default *background colour* is black but can be switched to white with ***V+W***, which also affects images output. Please note that writing transparent PNG images with a white background does not always provide good readability.

Displaying with 'thin' 1D results (i.e.: with a large number of cells) can sometimes be a bit dissatisfactory, toggling on the *'enhanced 1D'* display mode with ***V+1*** usually helps.

If a "TabF" result file was written, the *temperature at the bottom* can be displayed with ***V+K***.

Secondary windows can be *closed* with ***V+X***, meaning the colour-scale, virtual EDX, and scan-point windows.

7.2.8 Display.

The display of *length-scale* is toggled on and off by ***D+L***, the *reference length* can be set by default or chosen by the *user* with ***D+M***. Letting *Display MICRESS* select the length to be displayed automatically ensures that its representation is between one fifth and half of display. By default this scale is *horizontal* but it can also be flipped to *vertical* with ***D+F***.

Known limitation: the display of the length scale is not satisfactory with high zooming, but the results are anyway deemed not have much meaning at the corresponding resolutions.

The *zoom* can be called with ***D+Z***, the user then has to define the zoom box (area which will be displayed afterwards) by setting two (opposite) corners with mouse clicks, once these two points have been set, the zoom box is drawn, and can be refused by pressing the right mouse button or ***X*** (in which case another zoom box can be set), or accepted by pressing any other key. *Zoom out* with ***D+Y***, no progressive zooming out is done, i.e. zoom options are directly reset to their default values (i.e.: 'full picture'). It is also possible to *zoom back* with ***D+X*** (please note that only one set of zoom settings is saved…)

If the simulation set-up takes advantage on known symmetries or periodicities of the system and restricts the domain to part of the 'real space area', it is sometimes handy to display respectively *three, four or nine times the simulation domain*, with respectively ***D+3***, ***D+4***, ***D+9***. By default the 'copies' of domain are *mirrored* but they can also be *tranlsated* which can be toggled on and off with ***D+C***.

To allow readier positioning, a *grid* can be *displayed* with ***D+G***. The default number of subdivisions is 5, but this can be adjusted with ***D+H***.

Two additional display modes are available: *'RGB triangle'* and *'Miller Indices'* (respectively with ***D+T*** and ***D+I***): both are based on operations on the colour table, and can only be used for all the displayed results. The 'RGB triangle' mode, available with three solutions only, plots a composite of them, where the colour of a cell is the corresponding intensity of red, green and blue calculated from the displayed minimum and maximum. The Miller indices output of MICRESS® can also be colour-coded in the 'traditional' way (contribution of 001, 011 and 111 orientations). When these display modes are activated, the corresponding colour-scale is plotted in a secondary window under *Irix* and *Linux*, unfortunately not under *Windows* (a separate picture can be written out instead).

When two results are displayed, it is possible to display their *'difference'* with ***D+D***.

It is possible to use a *logarithmic scale* (***D+N***): the result data is first cut off to the maximum and minimum for the scale (which should be positive). It is also possible to take the *absolute value* of the results with ***D+A***.

7.2.9 'Vector field'.

Display MICRESS also supports *vector-field* representation (which can be activated with ***B+2***), the last file displayed being the 'Y' component of the vector, and the last-but-one the 'X' component (this is obviously only available with three files at least, when more are displayed, they get the same vector field). Similarly a *3D vector-field* mode is also available (***B+N***): the X, Y and Z components of the

vectors are respectively read from the last three files, the two ones in use depending on the cutting plane direction (the third one being temporarily ignored). The corresponding *settings* can be modified with ***B+S***: they are: the minimum and maximum intensity to be plotted, the 'thinning' distance: the averaging area for which a vector is displayed, and the position of the vector in this area: centred or not. A '*vector scale*' representing the maximal intensity can be plotted with ***B+X***. The *colour* of the vectors can be controlled with ***B+B***, which loops through black, white and bi-colour.

7.2.10 Isolines.

Display MICRESS supports various *isolines* options, the first of which is their *display*, which can toggled on and off with ***I+D***.

Automatic isolines: ***I+1...9***, automatically adds the corresponding number of isolines, equally spaced on the scale. Similarly, a *user-defined number of automatic isolines* can be added with ***I+N***.

User-defined isolines can be added with ***I+A***.

A single *isoline* can be *removed* with ***I+R***, and *all of them* with ***I+S***.

By default *isolines* are displayed with the *image* in the background, but this can be toggled on and off with ***I+C***. With the feature, only the *contours* are displayed (i.e.: only the isolines).

The values of the *isolines* currently displayed can be *printed* in the shell with ***I+V***.

To ensure that they can easily seen against any background, the isolines are by default black and white, this can be changed with ***I+B*** (*'bi-coloured' isolines*).

An *ASCII file* listing the coordinates of *'contour'* points for current time-step can be created with ***I+W***, and for *all outputs* with ***I+X***.

Note: if several result files are displayed the user will be prompted to select the files to which these operations should be applied to. Similarly to what is implemented for the scale, user-defined settings will affect all solutions which are selected simultaneously.

7.2.11 3D.

Display MICRESS can display 2D cuts (perpendicular to the main axis) of 3D simulations.

The *cutting plane* type, i.e. perpendicular to *X-axis*, *Y-axis* or *Z-axis* can be set respectively with ***3+X***, ***3+Y*** or ***3+Z***.

It is also possible to change the cutting plane position, by moving it *'up'* (increasing intercept coordinate), or *'down'* with ***3+U*** and ***3+D*** or *setting* the value with ***3+S***.

7.2.12 Outputs.

Display MICRESS supports image (various formats) and ASCII outputs. All these are done with current display settings (scale, colour representation, zoom parameters, etc.), and can be done for current time-step or batch-processed, meaning that they will be performed for all time steps.

Image output of current time-step: ***O+I***, of all time-steps: ***O+J***. ***O+L*** and ***O+H*** respectively request writing out of *'larger'* or *'high resolution'* images.

ASCII output can be written out with ***O+A*** and ***O+B*** (respectively without and with batch processing).

All the batch outputs have by default a name based on the *time-stamp* from the current *MICRESS* output, this can toggled on and off to *numbering* with ***O+N***.

An *image* of the *colour scale* only can be generated with ***O+C***. Please note that the orientation of this image depends on the orientation of the annotations.

The default *image driver* is *transparent background PNG* (*Portable Networks Graphic*), which can be selected with the keys ***O+T***, but can also be switched to *opaque background PNG* with ***O+O***, or *GIF* (*Graphics Interchange Format*) with ***O+G***, or *PostScript* with ***O+P***. Changing the image driver affects both images and 'Virtual EDX' outputs. The writing of '*PNG*' images is unfortunately not available under *Windows* (where the default image driver is '*GIF*').

The *default names* can be automatically accepted with ***O+D***.

7.2.13 'Virtual EDX'.

The *'Virtual EDX'* tool scans any given line from the display and plots the variation of the field variable along this line. It can be called by ***E+D***, after which the user is to set the beginning and end of the scan line with two mouse clicks, similarly to what is implemented for the zoom tool, the selected line is displayed on screen, and can be refused by pressing the right mouse button or ***X*** (in which case another line can be set), or accepted by pressing any other key. The results of the scan are then displayed in a secondary window.

It is also possible to display in a single plot the *scans* along the selected line for *all time-steps* with ***E+E***, or for a selection of outputs with ***E+C*** (*chosen time-steps*).

It is also possible to select lines parallel to the X or Y axis (of the display) respectively with (***E+X*** and ***E+Y***), the user can specify the line by entering the coordinate of the cut, similarly to what the *LineScan* tool does.

The last selected scan line can be plotted again with ***E+R*** (*replot*) or *re-scanned* with ***E+S***.

Scans can be *normalised* (rescaled so that their integral is one) with ***E+N***, which also disable it: (Also applies to all subsequent 'Virtual EDX' outputs).

Once a line has been set, it is possible to scan it for a given value over all the time-steps, this feature provides a convenient way of *tracking a front*, and can be called with ***E+F***. It gives the distance from the beginning of the scan line (first point selected) of the first occurrence of the set value, if this value is not found, -1 will be reported.

It is also possible to display the evolution over time of the value of the field variable for a given point with the *'Scan Point'* feature, which works in a very similar way to the 'Virtual EDX', it can be called with ***E+P***.

Note: if several result files are displayed the user will be prompted to select which solution(s) should be scanned. (This applies in a similar way to the 'Virtual EDX' outputs).

7.2.14 'Virtual EDX' outputs.

Text output for current time step creates an ASCII file with the results of the scan (***R+T***), it is also available *for all time steps* (***R+U***).

Scan position output writes an image with the position of the scan line: similarly *for current time step* (***R+I***), or *for all time steps* (***R+J***).

An image of the *curves* is also available respectively with ***R+C*** *for the current time step* and ***R+D*** *for all time steps*. It is also possible to generate a *single plot* with the scans for *all time-steps* with ***R+S***, or a *selection* of them, with ***R+M***.

For *'Front Tracking'*, *text output* (***R+F***) and *curve output* (***R+G***) are available, the corresponding scan position output are, of course, identical to the ones from 'Virtual EDX'.

Similarly for 'S*can Point'*, *text outputs* (***R+P***), *position output* (***R+Q***) and *curve output* (***R+R***) are available.

7.2.15 'Data information'.

The distance between two selected points can be displayed with ***W+M*** (*measure distance*). Similarly, the coordinates of a given point, along with the corresponding field values can be printed with ***W+C*** (*coordinates*).

Arbitrary *angles* can be *measured* with ***W+A***, angles with respectively with the *horizontal* or the *vertical* can be measured with ***W+H*** and ***W+V***.

The average, minimum and maximum from the current display are also available with ***W+E*** (*extrema*).

To compare ("*diff*") two *results*, press ***W+D***, the user is then prompted for a threshold value ('significant difference', allowing some numerical noise to be ignored). The same can also be applied sequentially to *all outputs* with ***W+F***.

A MICRESS® *'cell pointer'* can be pin-pointed with ***W+P***.

Information about the time when the last output was written and the *MICRESS®* and *Display MICRESS versions* can be printed out with ***W+I***.

Information about the *geometry* can be printed out with ***W+G***.

7.2.16 Remove output.

The current output can be *removed* from the displayed files with key ***K***. Please note that there is no 'undo' for this feature, the output is permanently removed from the file(s). Please note that a graphical interface to this feature is also available from the main interface (under '*Transfer MICRESS'*, '*Remove Outputs*').

7.2.17 Help.

Key ***H*** displays the summary of available options.

7.2.18 Exit.

To exit *Display MICRESS* press the right mouse button or ***X***.

7.2.19 Final remarks.

As previously mentioned, the graphical features of *Display MICRESS* are performed by the *PGPlot* library (www.astro.caltech.edu/~tjp/pgplot). The image output in *PNG* format (*Portable Network Graphics*) is made possible by the PNG library (www.libpng.orgl) and Z library (www.zlib.net). The *Z library* also handles compression (and decompression) of files, by calling its minimal implementation, *MiniGZip*. The 'screen driver' under *Windows* is from GrWin (http:/spdg1.sci.shizuoka.ac.jp/grwinlib/english). Please visit their home pages.

The first implementation of *Display MICRESS* was strongly inspired by the *PGPlot demo 4*.

Display MICRESS is not a commercial product, it is provided 'as is' on a courtesy basis.

Though *Display MICRESS* is convenient and pleasant to use it was unfortunately not actually meant to be a toy, therefore some apparent limitations result from a use that was simply not considered to be of interest to the post-processing of *MICRESS*® results, or even not intended altogether.

7.2.20 Summary of the shortcuts.

'Group'	Shortcut	Description
Time step	N	Display the next output.
	P	Go back to the previous output.
	L	Go to the last output.
	F	Go to the first output.
	M+N	Display the next output (dissociated).
	M+P	Go back to the previous output (dissociated).
	M+L	Go to the last output (dissociated).
	M+F	Go to the first output (dissociated).
Scale	S+M	User-defined min. and max. of the scale.
	S+R	User-defined 'range' (median value and range).
	S+D	Set min. and max. from display.
	S+G	Revert to 'global' min. and max.
	S+F	Force re-reading of the file to set min. and max.

Colour scale	C+1…11	Select the colour scale to be used.
	C+L	Loop though available colour scales.
	C+F	Fiddle with the brightness and contrast.
	C+R	Reset the brightness and contrast.
	C+I	Invert the colour scale.
	C+C	Cut-off the min. and max.
	C+S	Stepwise colour scale.
	C+U	User-defined steps for stepwise colour scale.
	C+T	Toggle between user-defined and default steps.
	C+K	Random stepwise colour scale.
Animation	A+R	Run animation.
	A+E	Animate to the end.
	A+S	Modify animation settings.
View	V+P	Reset number of panels
	V+F	Freeze panel.
	V+R	Redraw.
	V+Q	Auto-replot.
	V+S	Resize.
	V+Z	Auto-resize.
	V+A	Display annotations.
	V+C	Display the colour scale in a secondary window.
	V+O	Change the orientation of the annotations
	V+T	Increase 'thickness' of the colour scale.
	V+W	Change the background colour from black to white.
	V+1	Enhanced 1D display.
	V+K	Display the temperature at the bottom.
	V+X	Close secondary windows.

Display	D+L	Display length scale.
	D+M	Set length scale to be displayed.
	D+F	Flip length scale (horizontal to vertical).
	D+Z	Zoom in.
	D+Y	Zoom out.
	D+X	Revert to previous zoom settings.
	D+3	Three-folded symmetry.
	D+4	Four-folded symmetry.
	D+9	Nine-folded symmetry.
	D+C	Switch between mirror and translation symmetry.
	D+G	Display grid.
	D+H	Set number of grid lines.
	D+T	'RGB triangle' display.
	D+I	'Miller Indices' display.
	D+D	Display the 'difference' of two results.
	D+N	Logarithmic scale.
	D+A	Display absolute value of results.
'Vector field'	B+2	Vector-field display.
	B+3	3D vector-field display.
	B+S	Modify settings for vector-field display.
	B+X	Display 'vector scale'.
	B+B	Modify colour of vectors
Isolines	I+D	Display isolines.
	I+1...9	Add 1…9 automatic isolines.
	I+N	Add arbitrary number of automatic isolines.
	I+A	Add user-defined isolines.
	I+R	Remove an isoline.
	I+S	Remove all isolines.
	I+V	Print the values of the current isolines.
	I+B	'Bi-coloured' isolines.
	I+W	Write a list of the coordinates of 'contour' points.
	I+X	Same as above for all time-steps.
3D	3+X	Cutting plane type perpendicular to X-axis.
	3+Y	Cutting plane type perpendicular to Y-axis.
	3+Z	Cutting plane type perpendicular to Z-axis.
	3+U	Move cutting plane 'up'.
	3+D	Move cutting plane 'down'.
	3+S	Explicitly set cutting plane 'level' (intercept on axis).

Outputs	O+I	Write an Image output of current time-step.
	O+J	Write images output of each time-step.
	O+L	Toggle on and off writing of 'larger' images.
	O+H	Toggle on and off writing of 'high resolution' images.
	O+A	Write an ASCII output of current time-step.
	O+B	Write ASCII outputs of each time-step.
	O+N	Switch between time-stamp and numbering markers.
	O+C	Write an image of the colour scale.
	O+T	Write PNG images with transparent background.
	O+O	Write PNG images with opaque background.
	O+G	Write GIF (Graphics Interchange Format) images
	O+P	Write post-script images.
	O+D	Accept default names.
'Virtual EDX'	E+D	Display 'virtual EDX' scan for current time-step.
	E+E	Same as above for all time-steps.
	E+C	Same as above for a selection of time-steps.
	E+X	'Virtual EDX' on a line parallel to the X axis.
	E+Y	'Virtual EDX' on a line parallel to the Y axis.
	E+R	Re-plot scan line.
	E+S	Re-scan scan line.
	E+N	Toggle on and off normalising the scans.
	E+F	'Front-tracking'.
	E+P	'Scan-point'.
'Virtual EDX outputs'	R+T	Text output for current time step.
	R+U	Text output for all time steps.
	R+I	Scan position output for current time step.
	R+J	Scan position output for all time steps.
	R+C	Image of the curve(s) for the current time step.
	R+D	Images of the curve(s) for all time steps.
	R+S	Image of the curves for all time steps.
	R+M	Image of the curves for a selection of time steps.
	R+F	'Front Tracking' text output.
	R+F	'Front Tracking' curve output.
	R+P	Scan-point' text output.
	R+Q	Scan-point' position output.
	R+R	Scan-point' curve output.

'Data information'	W+M	Measure distance.
	W+C	Print coordinates and field value(s) for a point.
	W+A	Measure angle.
	W+H	Measure angle with the horizontal.
	W+V	Measure angle with the vertical.
	W+E	Print average, and extrema from the current display.
	W+D	Compare two files for the current time-step.
	W+F	Compare two files for all time-steps.
	W+P	Pin-point 'cell pointer'.
	W+I	Print information about MICRESS® version.
	W+G	Print information about the geometry.
Remove output	K	Remove current time-step from output file(s).
Help	H	Display the summary of available options.
Exit	X	Exit.

7.3 Libraries used by MICRESS and Display_MICRESS.

Copyright notice of libraries used by MICRESS and *Display MICRESS*.

7.3.1 Copyright notice of zlib (MICRESS and Display_MICRESS).

zlib.h -- interface of the 'zlib' general purpose compression library version 1.1.3, July 9th, 1998

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The data format used by the zlib library is described by RFCs (Request for Comments) 1950 to 1952 in the files ftp://ds.internic.net/rfc/rfc1950.txt (zlib format), rfc1951.txt (deflate format) and rfc1952.txt (gzip format).

7.3.2 Copyright notice of PGPlot (Display_MICRESS).

```
*****************************************************************************
*                    PGPLOT Fortran Graphics Subroutine Library             *
*                                 Version 5.2.2                             *
*****************************************************************************

*****************************************************************************
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*            Pasadena, California 91125, USA                                *
*                                                                           *
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*                                                                           *
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*****************************************************************************
```

7.3.3 Copyright notice of libPNG (Display_MICRESS).

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Kevin Bracey
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8 Installing MICRESS®.

8.1 Installing MICRESS® under Windows™.

MICRESS® and *DP_MICRESS* require very little installation work, which should anyway be handled by the installation script, but some users might be interested in performing these tasks themselves (for example when installing without administrator privileges), or simply knowing what's been performed on their behalf.

8.1.1 Overview:

The following topics are going to be addressed in the present document: first of all, a quick overview of the contents of the "*MICRESS®* Bin directory". Then a few words about the installation of *MICRESS®*: how to start a simulation by right-clicking a driving file ("Contextual Menu"), and how to add the "Bin" to your path, so that *MICRESS®* and *DP_MICRESS* can be conveniently called from the command-line. Finally the tasks related to *DP_MICRESS* will be discussed: how to create the file type for the binary result files, and associate it, as well as a description of the settings.

- *Privileges:*
  The same privilege restrictions as for the installation script apply: administrator privileges are necessary for the following to apply to all users logging on the machine, but any user should be able to that for him- or herself (depending on the local Windows settings).
- *Windows version, language:*
  The following step-by-step descriptions match what has to be done with an English version of *Windows XP*, but this process is very similar with any other *Windows* flavour. The name of the settings will certainly be different if your operating system is in another language, but the features are nevertheless the very same ones.
- *Final warning:*
  Please note that, the following should not be construed in any respect as the best or the easiest way of performing the corresponding tasks, just what looked to us to be the most obvious one, and it happens to work!

8.1.2 Contents of the 'Bin' directory:

This is where the *MICRESS®* binaries and their related files are stored:

- *MICRESS.exe: MICRESS®* binary.
- *tq.dll: Thermo-Calc™'s TQ* interface dynamic load library (only necessary if you have a *TQ-coupled MICRESS®* version). (Please note that '**.dll*' files might be automatically hidden by *Windows Explorer*).
- *DP_MICRESS.exe* post-processing tool for *MICRESS®* (bundled with its graphical front-end).
- *DP_MICRESS_Data* Display_MICRESS core (…).
- *DP_MICRESS_Settings.txt* text file storing user settings for *DP_MICRESS* (which will be discussed further on).

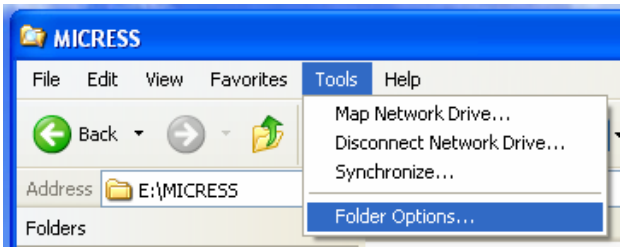
8.1.3 Installing MICRESS®:

The *MICRESS®* binaries are rather self-contained and do not require much further processing than simply copying them on your system, but a few steps might turn out to be of interest.

⇨ *Thermo-Calc ™'s TQ interface:*

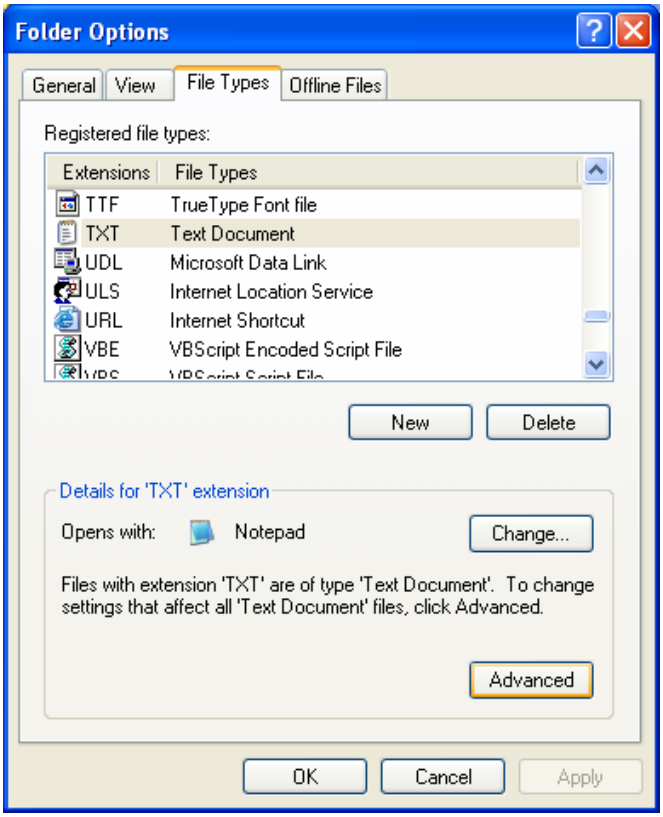
It is recommended that you keep the *MICRESS.exe* and *tq.dll* files together, which ensures that *MICRESS™* can find the *TQ* library, a link to *MICRESS.exe* can be placed where you need it, if need be.

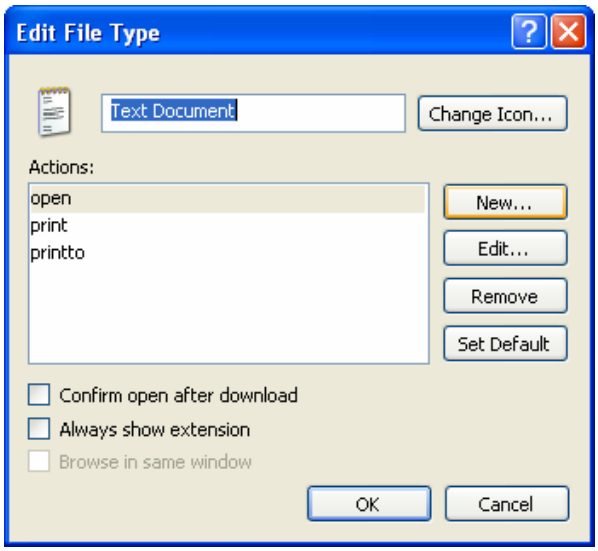
⇨ *Contextual menu (starting MICRESS® by right-clicking a driving file):*

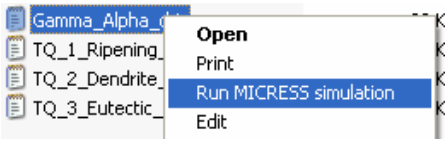


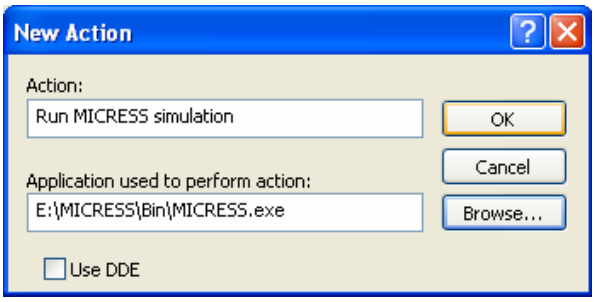
While a driving file (which is a text file, and therefore typically has the ".txt" extension) should stay associated with your favourite text editor, it is sometimes convenient to start *MICRESS®* by right-clicking it, therefore dispensing of the need of dragging-and-dropping it on the binary (or a link to it).

This can be quite easily done by editing the file association for text files: open *Windows Explorer* and click on the "Tools" and "Folder options…", then go to "File Types", select "Text Document" and click "Advanced". In the "Edit File Type" dialog, add a new "Action", called "Run MICRESS simulation" (for example) pointing to your *MICRESS®* binary, and click "OK", once more "OK" and "Apply": you can now run a simulation by right clicking on a driving file a selecting "Run MICRESS simulation".


Folder Options
General View File Types Offline Files
Registered file types:
Extensions File Types
TTF TrueType Font file
TXT Text Document
UDL Microsoft Data Link
ULS Internet Location Service
URL Internet Shortcut
VBE VBScript Encoded Script File
New Delete
Details for 'TXT' extension
Opens with: Notepad
Change...
Files with extension 'TXT' are of type 'Text Document'. To change settings that affect all 'Text Document' files, click Advanced.
Advanced
OK Cancel Apply



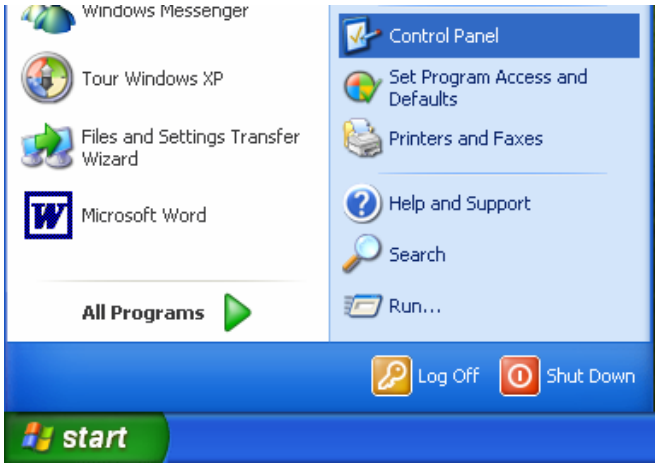


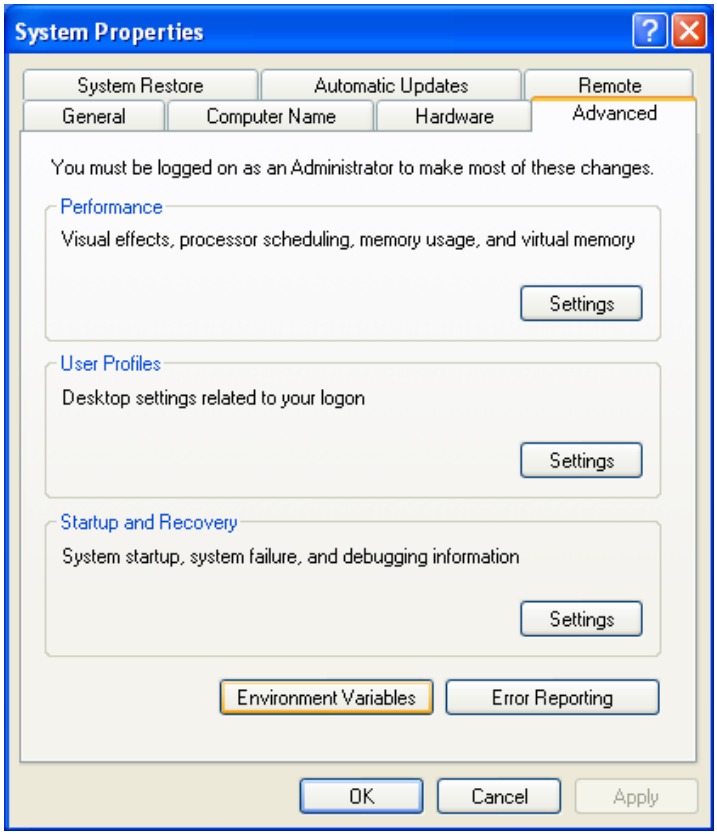


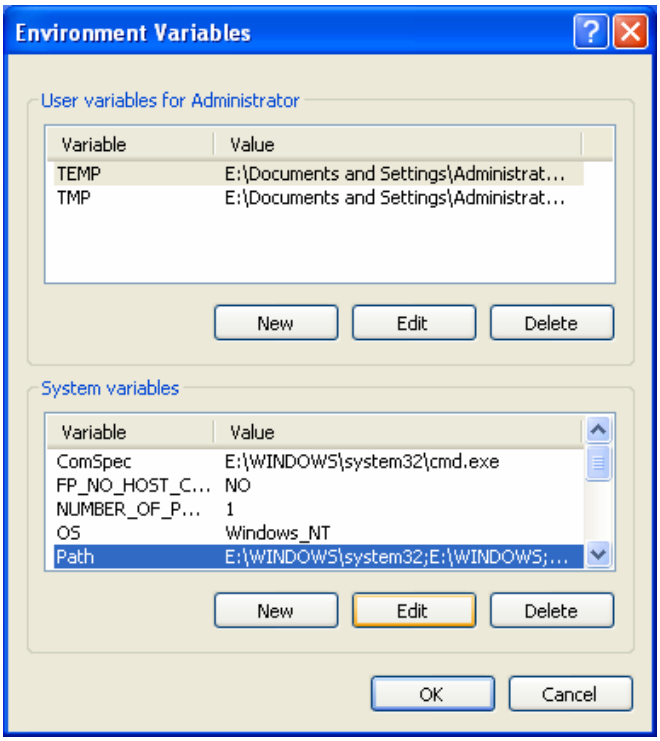
⇨ *Adding the MICRESS® 'Bin directory' to your path:*

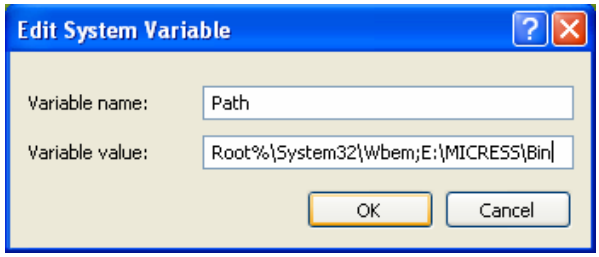
This is only useful if you plan to start MICRESS™ or DP_MICRESS from the command-line, in which case not having to specify the path to the binaries can save quite a bit of typing (i.e.: "MICRESS" instead of "E:\MICRESS\Bin\MICRESS" for example).

In the Windows "Control Panel", go to "System" (possibly via "Performance and Maintenance" if the "Category View" is enabled), and go to "Advanced" and select "Environment Variables". From there, edit the "System Variable" named "PATH", to which the absolute path to your "Bin directory" should be appended (with a semi-column ";" as an item separator).









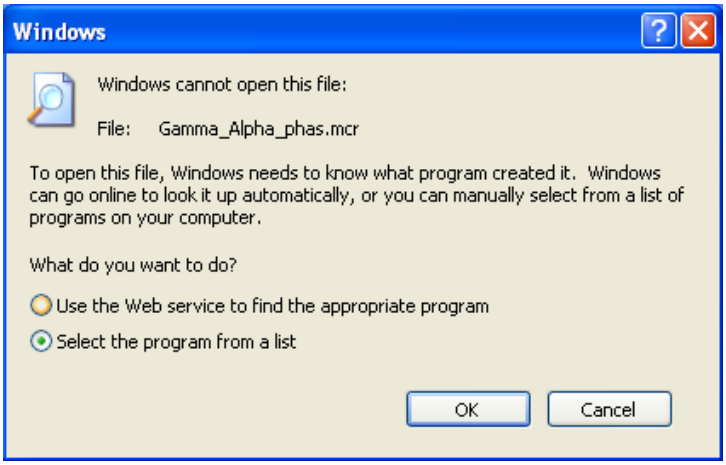
8.1.4 Installing DP_MICRESS:

⇨ *Associate MICRESS result file extension with DP MICRESS:*

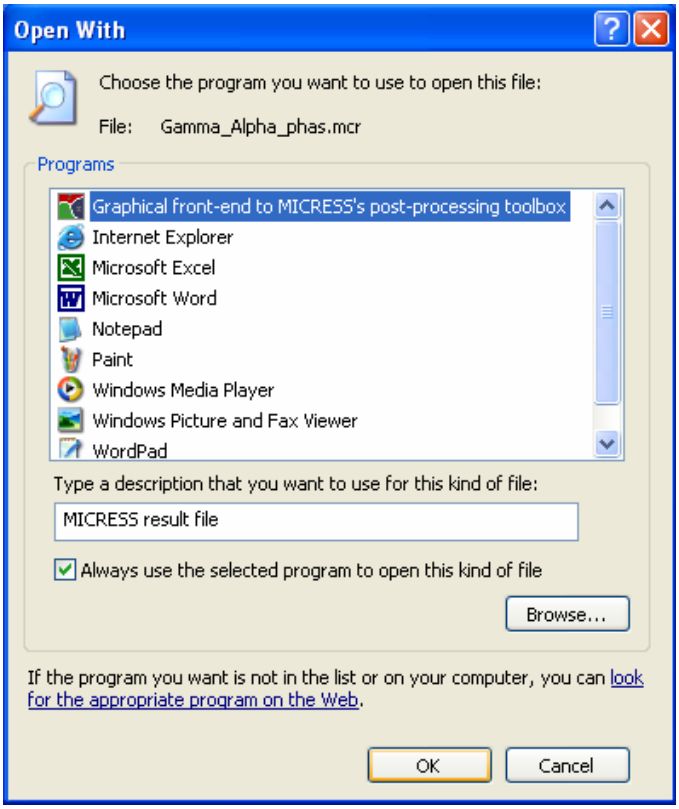
If an "Mcr File Type" is already present on your system, proceed in a similar way as described in "*Contextual menu (starting MICRESS® by right-clicking a driving file)*".

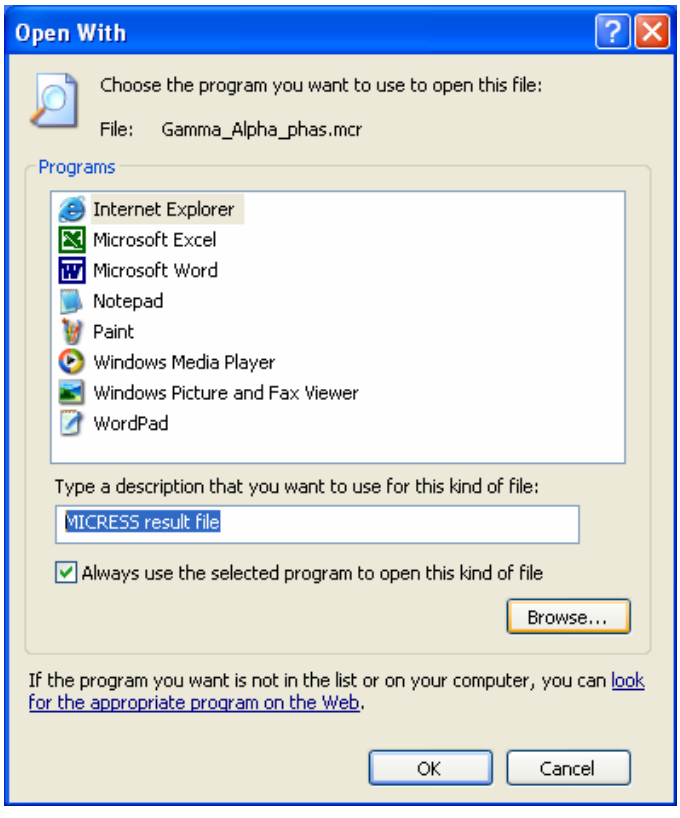
Gamma_Alpha_conc1.mcr 18,001 KB MCR File
Gamma_Alpha_conc2.mcr 18,001 KB MCR File
Gamma_Alpha_geoF.mcr 1 KB MCR File
Gamma_Alpha_phas.mcr 18,001 KB MCR File

Otherwise, double-click a binary result file: Windows will own up that there is no defined way of dealing with such files, choose "Select the program from a list". In the following dialog, a description can be entered, such as "MICRESS result file", click on "Browse" to select the *DP_MICRESS* binary, accept it with "OK" (twice).


Windows
Windows cannot open this file:
File: Gamma_Alpha_phas.mcr
To open this file, Windows needs to know what program created it. Windows can go online to look it up automatically, or you can manually select from a list of programs on your computer.
What do you want to do?
Use the Web service to find the appropriate program
Select the program from a list
OK
Cancel

The file association has now been created, and simply double-clicking a *MICRESS®* result file will start *DP_MICRESS*. Please note that *DP_MICRESS* will be called the default settings (a single result, binary file not compressed, etc...), if you wish to use other settings, double-click a 'geoF' file, which will call instead the front-end for calling *Display_MICRESS*.


Open With
Choose the program you want to use to open this file:
File: Gamma_Alpha_phas.mcr
Programs
Graphical front-end to MICRESS's post-processing toolbox
Internet Explorer
Microsoft Excel
Microsoft Word
Notepad
Paint
Windows Media Player
Windows Picture and Fax Viewer
WordPad
Type a description that you want to use for this kind of file:
MICRESS result file
Always use the selected program to open this kind of file
Browse...
If the program you want is not in the list or on your computer, you can look for the appropriate program on the Web.
OK
Cancel


Open With
Choose the program you want to use to open this file:
File: Gamma_Alpha_phas.mcr
Programs
Internet Explorer
Microsoft Excel
Microsoft Word
Notepad
Paint
Windows Media Player
Windows Picture and Fax Viewer
WordPad
Type a description that you want to use for this kind of file:
MICRESS result file
Always use the selected program to open this kind of file
Browse...
If the program you want is not in the list or on your computer, you can look for the appropriate program on the Web.
OK
Cancel

Gamma_Alpha_conc1 18,001 KB MICRESS result file
Gamma_Alpha_conc2 18,001 KB MICRESS result file
Gamma_Alpha_geoF 1 KB MICRESS result file
Gamma_Alpha_phas 18,001 KB MICRESS result file

⇨ *Settings file:*
It is possible to customise several things via the settings file (*'DP_MICRESS_Settings.txt'*).
If you want to access *Display_MICRESS* manual and / or the MICRESS hotline from *DP_MICRESS*, set respectively *'Display_Manual'* and *'Display_Link'* to *'1'*. In this case *'Acrobat'* and *'Browser'* should be set to (absolute) paths to a suitable Portable Data File viewer and web browser. Similarly an external snapshot tool can also be made available.
The front-end for calling DP_MICRESS is available in two flavours: cut-down and advanced: switch between the two with "Standard_Only". Some additional flags can also be passed on to *Display_MICRESS* each time it is called.

DP_MICRESS_Settings.txt

```
#
########################################
#                                      #
#              Settings                #
#                                      #
########################################
#
Default_GUI              : 1
Docking                  : 1
#
Display_Manual           : 0
Acrobat                  : P:\Acrobat\Reader\AcroRd32.exe
#
Display_Link             : 0
Browser                  : P:\Mozilla Firefox Firefox.exe
#
Display_Snapshot_Tool    : 0
Snapshot_Tool            : snapshot.exe
#
Standard_Only            : 1
Additional_Flags         : 0
#
```

8.2 Installing MICRESS® under UNIX.

This section was mostly added for symmetry's sake, as installing ***MICRESS®*** and *DP_MICRESS* under Unix (and Linux) is straightforward.

The user should make sure that Thermo-Calc™'s TQ-interface library can be picked-up. (If you do not intent to use TQ-coupled binaries this step can obviously be skipped). To check that the easiest is to use the 'ldd' command which should return something similar to the following. If not the 'LD_LIBRARY_PATH' environment variable can be extended to include a directory where your 'libtq.so' is, or it can be copied (or a link to it) can be placed in a directory already searched for this purpose.

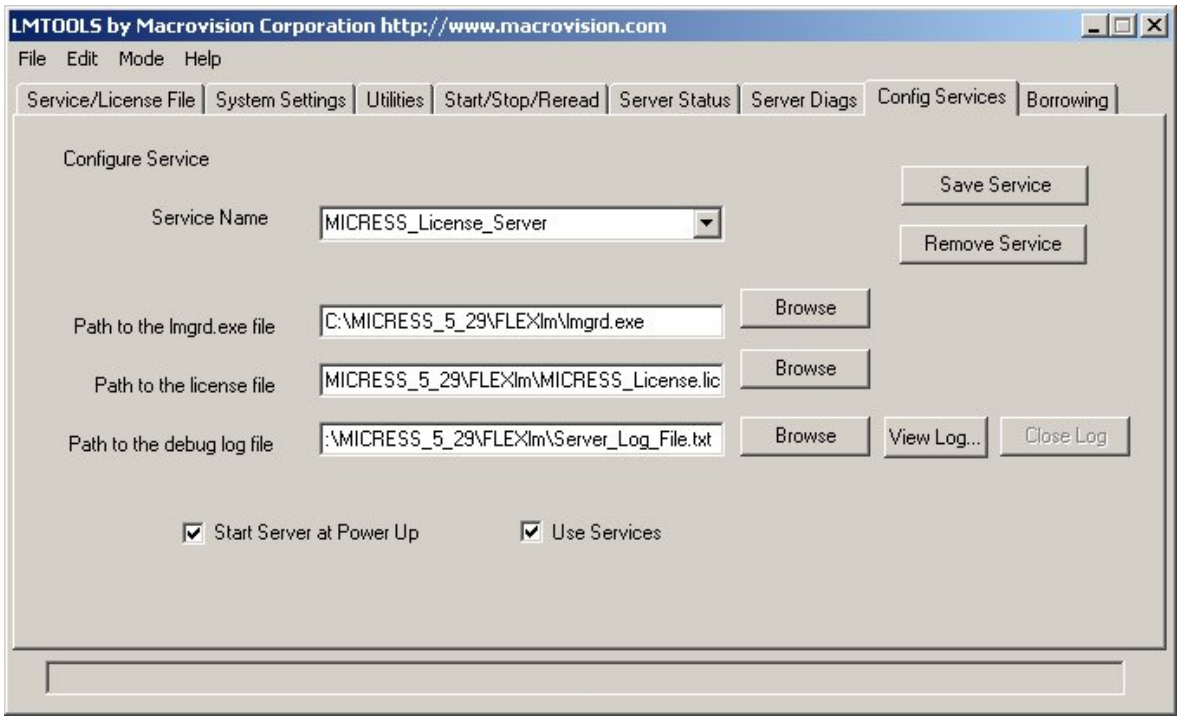
Command-line

```
ldd MICRESS
    linux-gate.so.1 =>  (0xffffe000)
    libpthread.so.0 => /lib/tls/libpthread.so.0 (0x4002d000)
    libtq.so => /usr/local/lib/libtq.so (0x4003e000)
    libc.so.6 => /lib/tls/libc.so.6 (0x450f4000)
    libm.so.6 => /lib/tls/libm.so.6 (0x45209000)
    /lib/ld-linux.so.2 => /lib/ld-linux.so.2 (0x40000000)
```

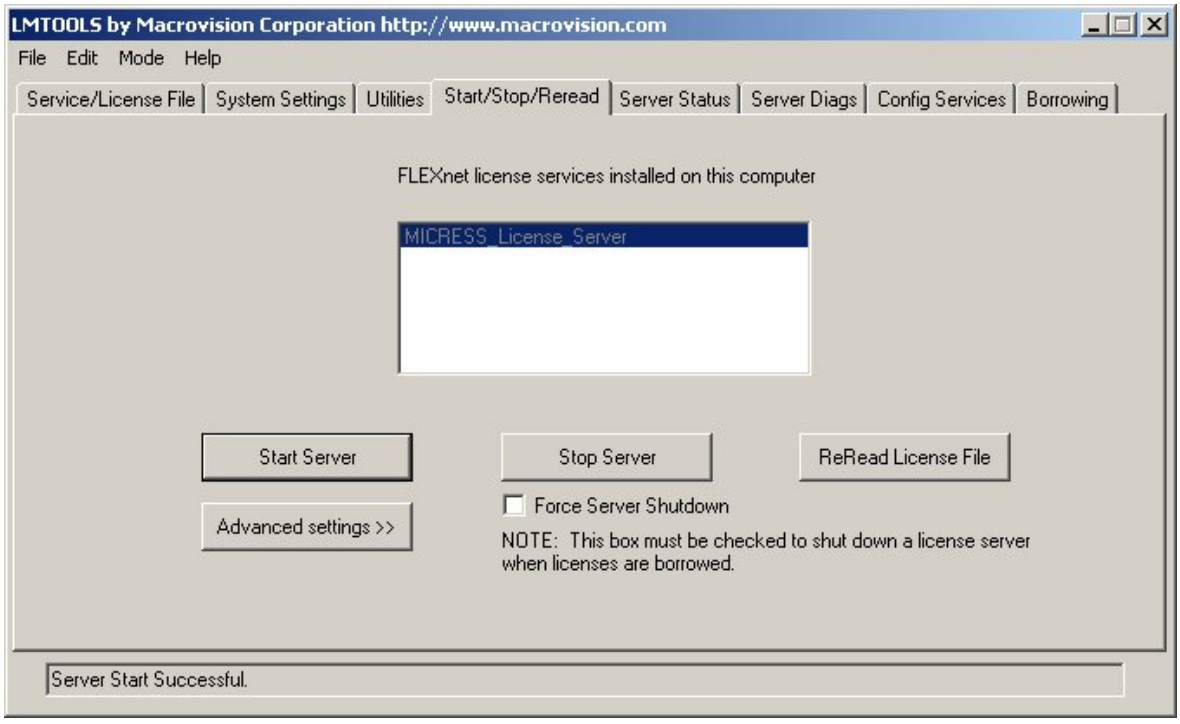
It can prove convenient to add the MICRESS bin directory to your path (to save some typing), or place links to MICRESS and DP_MICRESS in a directory in your search path.
The DP_MICRESS settings file can also be edited in similar manner as mentioned before.

8.3 Starting a FLEXlm™ license server under Windows™.

Start 'lmtools.exe' and go to the 'Config Services' tab (last but one), and set it up in a similar way as shown here (this is rather self-explanatory); once this is done, save this 'Service'.



Afterwards, witch to the 'Start/Stop/Reread' tab (roughly in the middle), pick the service you have just saved, and start it.



9 Standard examples.

Some examples are provided with MICRESS®, unfortunately they cannot cover the whole scope of the software, but should nevertheless cover some typical cases, and can be used as starting points for other purposes.

9.1 Aluminium copper.

The '*AlCu_dri*' and '*AlCu_Equiaxed_dri*' examples are concentration-coupled with Thermo-Calc™ coupling, of a binary aluminium copper alloy. They are both dendritic, the first one corresponding to a directional solidification, and the second to an equiaxed one. The second one also provides an example of the use of the 'seed-density' nucleation model.

9.2 Delta-gamma.

'*Delta_Gamma_dri*' is a simulation of a ternary steel model alloy (iron, carbon and manganese), simulating a dendritic $\delta \rightarrow \gamma$ transformation. It is also coupled to Thermo-Calc™. Both are concentration-coupled.

9.3 Gamma-alpha.

A series of examples ('*Gamma_Alpha_dri*', '*Gamma_Alpha_TQ_dri*' and '*Gamma_Alpha_Stress_dri*') simulating the $\gamma \rightarrow \alpha$ transformation for a ternary steel model alloy (iron, carbon and manganese). The first two are mostly intended as a comparison of the use of MICRESS® with and without coupling to Thermo-Calc™. Both are concentration-coupled. The third one shows how the coupling to stress field can be added (this example is also 3D).

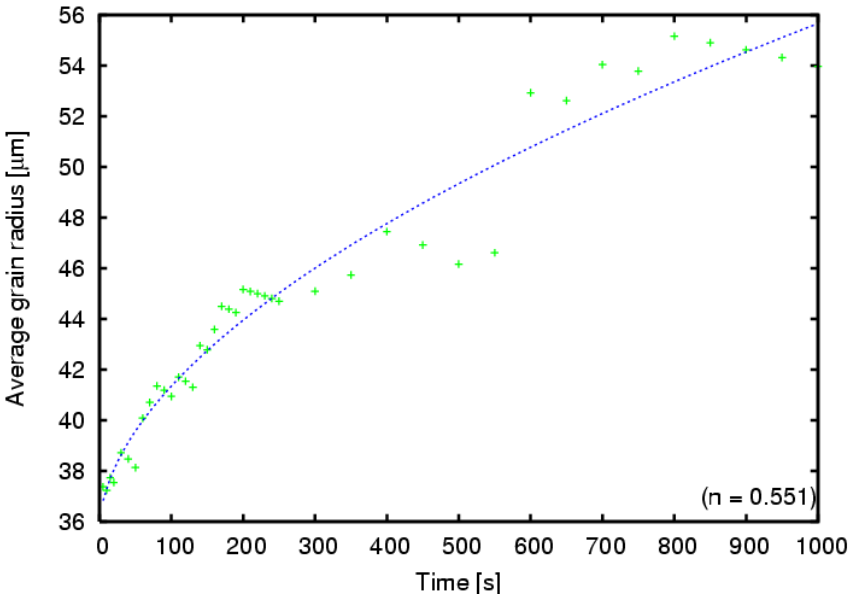
9.4 Grain growth.

These four examples, '*Grain_Growth_dri*', '*Grain_Growth_Particle_Pinning_dri*', '*Grain_Growth_Solute_Drag_dri*' and '*Grain_Growth_Solute_Drag_KTH_dri*' show how MICRESS® can be used without coupling to external fields, i.e.: 'only' phase-field. These examples show the use of a read-in initial microstructure (see paragraph 10.3). The first one displays 'pure' grain-growth whereas the other ones show respectively examples of the particle-pinning [6], solute-drag [7], and KTH-solute-drag [14] models. The mobility data for the '*Grain_Growth_Solute_Drag_KTH_dri*' was kindly provided by H. Strandlund from material for [14].

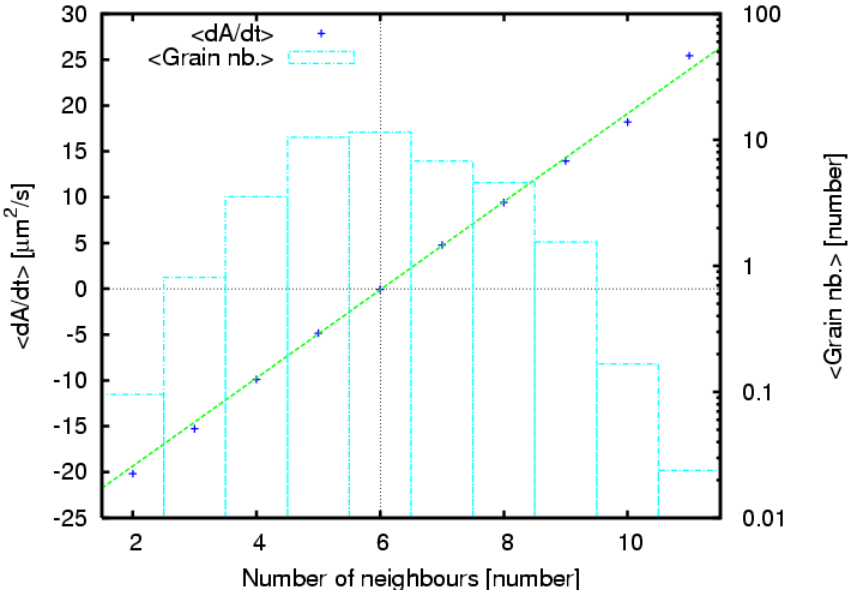
The micrograph used to create the initial microstructure is courtesy of IEHK, RWTH Aachen.

The 'pure' grain-growth example can readily be used to validate the settings by checking that the growth-rate exponent is close to the theoretical value, as well as that the von Neumann-Mullins relation is fulfilled.

Growth rate exponent: the evolution of the average grain radius over time. The data was fitted with a least-squares method using $\langle R \rangle(t) = \langle R \rangle(t_o) + k \times (t - t_0)^m$ (where $t = t_0$): the resulting growth rate exponent m was **0.551** which agrees quite well with the theoretical prediction of 0.5. The staggered and fluctuating look of the curve from 200 s on is due to the relative paucity of the statistics (only 53 grains, and less than 40 from then on).



The ***Von Neumann-Mullins relation*** states that the growth rate of a grain is proportional to its number of sides $\frac{dA}{dt} = \gamma \times m \times \frac{\pi}{3} \times (n - 6)$, where A is the area of a grain, γ the surface tension, m the interface mobility and n the number of sides. The number of neighbours of a grain was used as a proxy for its number of sides. The grains where sorted into classes according to their number of neighbours and the derivative of the surface was then averaged per class. The data was fitted with a least-square method weighted with the class population: the correlation coefficient was r = 0.9997, and the predicted 'stable configuration' was 6.024 neighbours, which is in accordance with the theory.



9.5 'Phosphorus peak'.

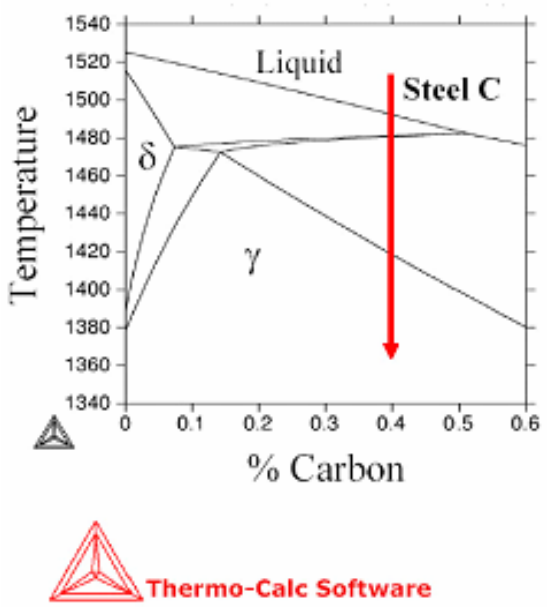
These two examples, 'P_Peak_1D_dri' and 'P_Peak_2D_dri' show full multicomponent diffusion with coupling to Thermo-Calc™ on an industrial steel. The first is one-dimensional and provides a ready benchmark against DICTRA™.

The work summarised hereafter was supported by the European Community through the VESPISM project (contract G5RD-CT-2000-00315).

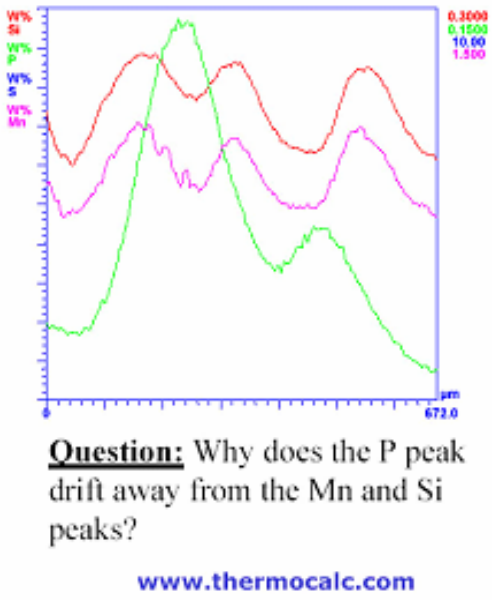
The following material marked "Thermo-Calc" is courtesy of Thermo-Calc Software AB. (www.thermocalc.com), and the material marked "Corus" is courtesy of Corus Group plc., Swinden Technology Centre (www.corusgroup.com).

9.5.1 Initial observation.

These simulations stem from the observation of micro-segregation profiles at the Swinden Technology Centre of Corus, which show an unusually clear case of "phosphorus-peak drift". The investigation of this process was performed by Thermo-Calc Software AB. using DICTRA™. The simulation could later be repeated with MICRESS®, both in 1D and 2D.

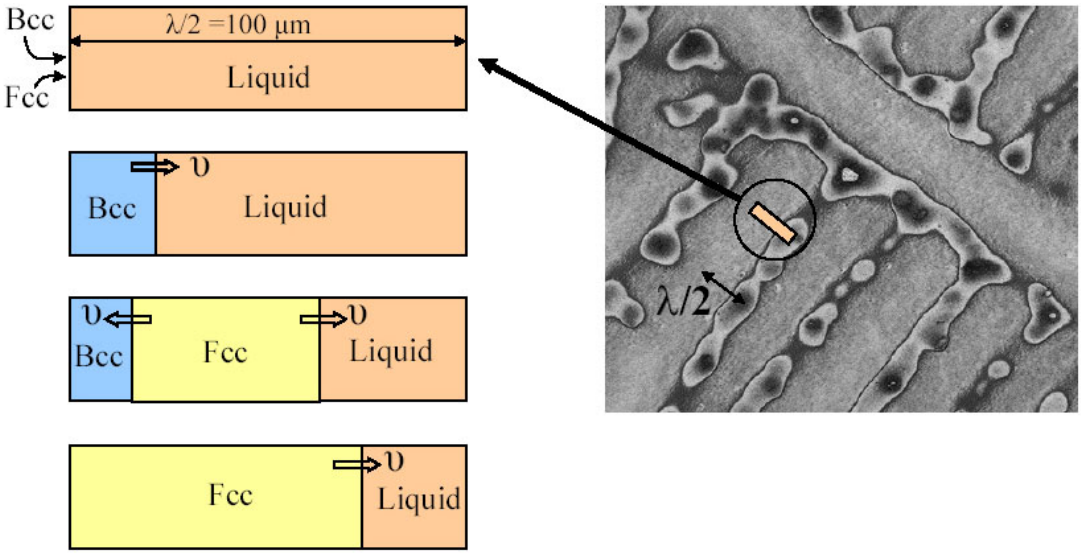


Courtesy of Thermo-Calc Software AB.



Courtesy of Corus

9.5.2 Simulation set-up.

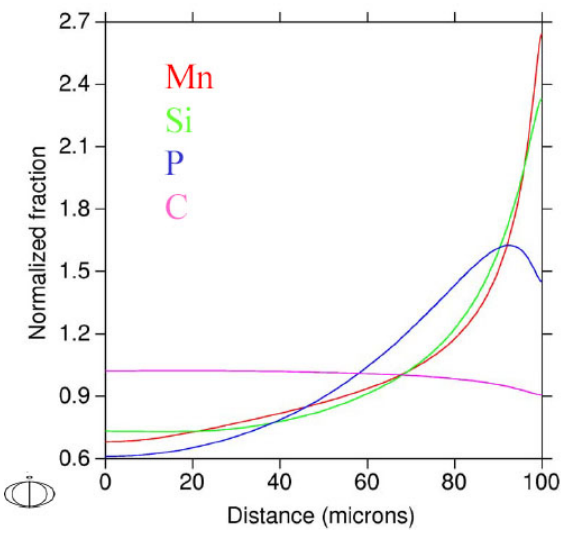


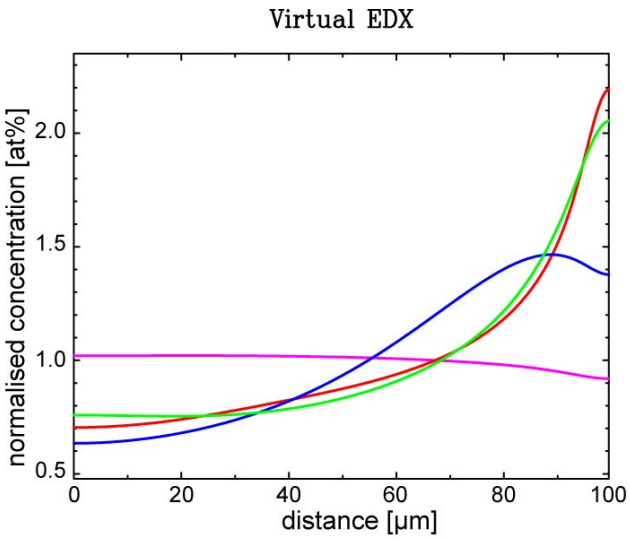
- Secondary dendrite arm spacing assumed to be 200 µm.

Thermo-Calc Software www.thermocalc.com

Courtesy of Thermo-Calc Software AB.

9.5.3 *T ≈ 1660 K, a*fter the last liquid disappears.



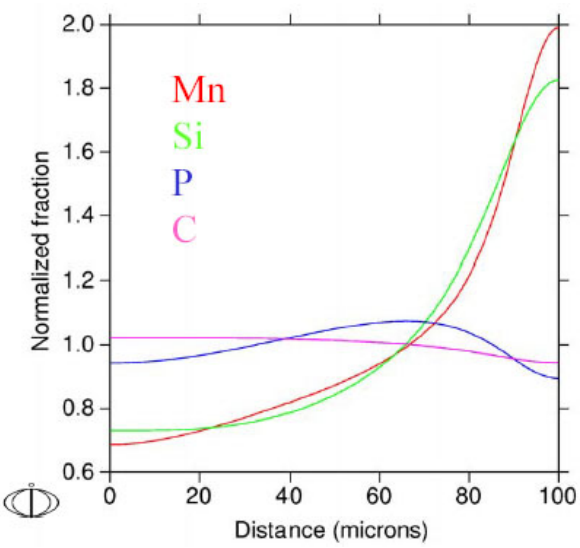


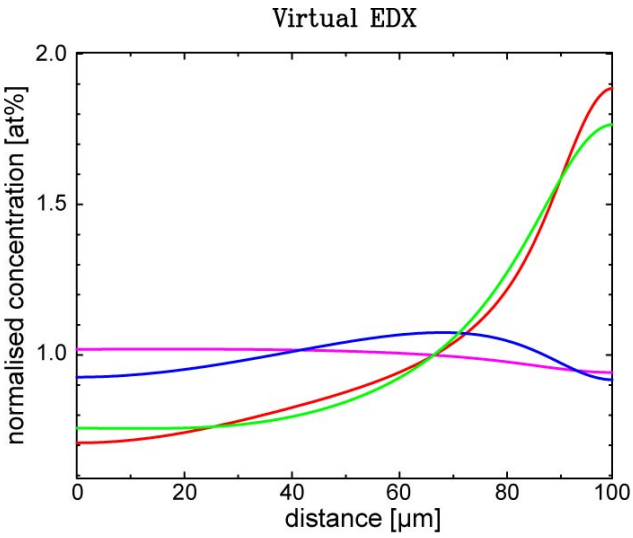
Simulated with DICTRA™.

Simulated with MICRESS®

Courtesy of Thermo-Calc Software AB.

9.5.4 *T ≈ 1580 K.*



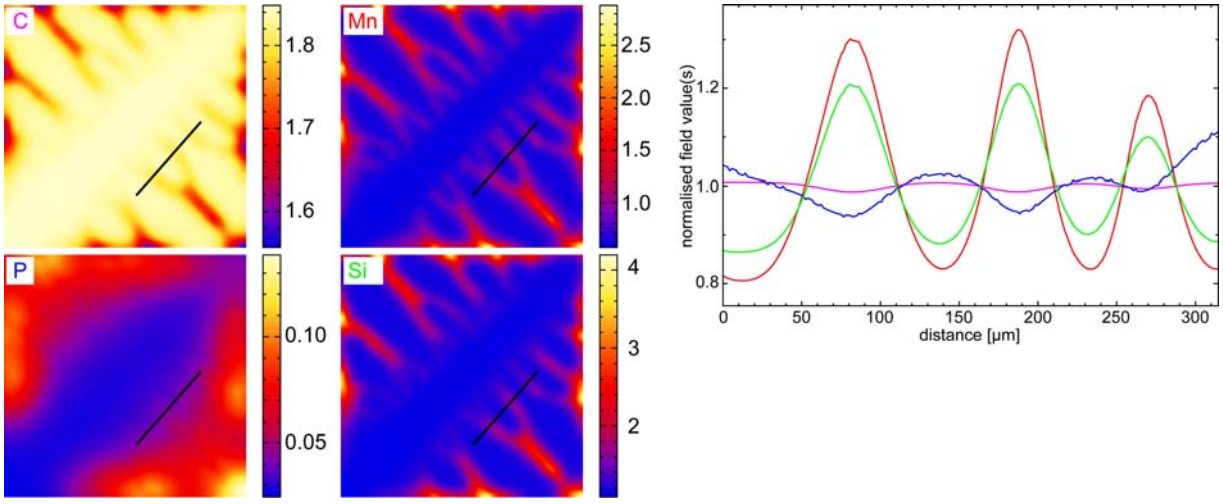


Simulated with DICTRA™.

Simulated with MICRESS®

Courtesy of Thermo-Calc Software AB.

9.5.5 *2D, T ≈ 1365 K.*



9.6 Recrystallisation.

These five examples, ‘ReX_1_dri’, ‘ReX_2_dri’, ‘ReX_3_dri’, ‘ReX_4_dri’, and ‘ReX_5_dri’ illustrate various topics related to recrystallisation: such as the influence of misorientation and stored-energy on growth, ‘nucleation’ and sub-grain model.

9.7 Strees.

‘Stress_dri’ shows the simulation of Eshelby's solution.

9.8 Basic TQ-coupling.

Two examples, ‘TQ_Ripening_dri’ and ‘TQ_Eutectic_dri’ illustrate the basics of the Thermo-Calc™ coupling (via its TQ interface). The simulate phase transformations in an aluminium silver alloy. The first one is isothermal and shows the effect of curvature. The second is similar and adds heat extraction and simulation of release of latent heat, with growth of a primary and secondary phase, as well as solid-solid interaction after complete solidification.

9.9 Temperature.

‘Temperature_dri’ illustrate the use of coupling to temperature field (growth of sphere in an undercooled liquid).

10 Fully Answered Questions.

10.1 Reading MICRESS results.

More than a full description of the output format, which is bound to be incomplete, here is a brief description of the files contents, as well as code snippets implementing reading of geometry file and one 'output' of a result file. These examples are limited to Fortran and Perl, which happen to be the only languages we currently actively use to manipulate MICRESS files. A C implementation would certainly also be handy, but should be straightforward to adapt from the Perl one. These examples are 'barebones', without any checks or error handling whatsoever.

They also apply to reading 'uncompressed' files (which is not the default!): it is left to the user to deal with this: by reading compressed results all the same (trivial in Perl with the use of the 'Compress::Zlib' module, freely available form the CPAN repository for example), calling the ZLib library to do the conversion, uncompressing the results before reading them (Display_MICRESS can do it, for example), or disabling compression.

10.1.1 Anatomy of MICRESS® results files.

The results files are binary sequential files written by a fortran program: if read by a program written in another language, the 'record length' should correspondingly be dealt with: it is a 4-bytes integer (storing the length of the record in bytes).

They are written in 'native' format, i.e. 'little-endian' on platforms using Intel-compatible processors, and 'big-endian' otherwise.

The 'geoF-file' store information about the geometry: they consist mostly of one fortran 'record' storing the number of points in the X, Y and Z directions, followed by the grid spacing in centimetres in these three directions (which happen to be identical). The numbers of points are 4-bytes integers, and the grid spacing 4-bytes reals.

The result files store the field value for a given output-time, a record for each. First the time (4-bytes real), then the number of points in the simulation domain (a 4-bytes integer which is the product of the number of points in the X, Y and Z directions), followed by the field values for each cell, that is 'number of points' 4-bytes reals. They are ordered in the following way: first all the values for X, Y=1 and Z=1, then the same for Y=2 (if applicable) and so on, afterwards for Z=2 and so on…

10.1.2 In Fortran.

```
!
!      [...]
!
       INTEGER             ::   Nb_Pts_X, Nb_Pts_Y, Nb_Pts_Z, Nb_Points
       INTEGER             ::   x, y, z
!
       REAL                ::   Grid_Spacing_X, Grid_Spacing_Y
       REAL                ::   Grid_Spacing_Z, Time
       REAL, ALLOCATABLE   ::   Result_Data(:,:,:)
!
!      [...]
!
! Open 'GeoF' file
! ----------------
!
       OPEN ( UNIT = Unit_GeoF, FILE = TRIM(GeoF_File_Name),             &
      &   FORM = "UNFORMATTED", ACTION = "READ", ACCESS = "SEQUENTIAL", &
      &                                 STATUS = "OLD", IOSTAT = IO_Stat )
!
!      [...]
!
! Read from 'GeoF' file
! ---------------------
!
       READ ( UNIT = Unit_GeoF, IOSTAT = IO_Stat ) Nb_Pts_X, Nb_Pts_Y,  &
      &          Nb_Pts_Z, Grid_Spacing_X, Grid_Spacing_Y, Grid_Spacing_Z
!
!      [...]
!
! Open result file
! ----------------
!
       OPEN ( UNIT = Unit_Result, FILE = TRIM(Result_File_Name),         &
      &   FORM = "UNFORMATTED", ACTION = "READ", ACCESS = "SEQUENTIAL", &
      &                                 STATUS = "OLD", IOSTAT = IO_Stat )
!
!      [...]
!
! Read from result file
! ---------------------
!
       READ ( UNIT = Unit_Result, IOSTAT = IO_Stat ) Time, Nb_Points,   &
      &                    ( ( ( Result_Data(x,y,z), x = 1, Nb_Pts_X ), &
      &                                 y = 1, Nb_Pts_Y ), z = 1, Nb_Pts_Z )
!
!      [...]
!
```

10.1.3 In Perl.

```
# Open 'GeoF' file
# ----------------
#
  if ( ! open ( GEOF, "<", $GeoF_File_Name ) ) {
    print "Error while opening: " . $GeoF_File_Name . "\n (" . $^E . ")\n\n";
    exit;
  };
  if ( ! binmode ( GEOF ) ) {
    print " Error while setting file to 'binmode': " . $GeoF_File_Name
          . "\n (" . $^E . ")\n\n";
    close ( GEOF );
    exit;
  };
#
# [...]
#
# Read from 'GeoF' file
# ---------------------
#
  if ( read ( GEOF, $Bytes, 32 ) != 32 ) {
    print " Error while reading from: " . $GeoF_File_Name . "\n (" . $^E
          . ")\n\n";
    close ( GEOF );
    exit;
  };
  ( $Record_Length_1, $Nb_Pts_X, $Nb_Pts_Y, $Nb_Pts_Z, $Grid_Spacing_X,
    $Grid_Spacing_Y, $Grid_Spacing_Z, $Record_Length_2 )
    = unpack ( "I4f3I", $Bytes );
#
# [...]
#
# Open result file
# ----------------
#
  if ( ! open ( RESULT, "<", $Result_File_Name ) ) {
    print "Error while opening: " . $Result_File_Name . "\n (" . $^E
          . ")\n\n";
    exit;
  };
  if ( ! binmode ( RESULT ) ) {
    print " Error while setting file to 'binmode': " . $ Result _File_Name
          . "\n (" . $^E . ")\n\n";
    close ( RESULT );
    exit;
  };
#
# [...]
#
# Read from result file
# ---------------------
#
  $Nb_Pts = $Nb_Pts_X * $Nb_Pts_Y * $Nb_Pts_Z;
  $Bytes_to_Read = 4 * ( $Nb_Pts + 4 );
  $Format = "IfIf" . $Nb_Pts . "I";
  if ( read ( RESULT, $Bytes, $Bytes_to_Read ) != $Bytes_to_Read ) {
    print " Error while reading from: " . $Result_File_Name . "\n (" . $^E
          . ")\n\n";
    close ( RESULT );
    exit;
  };
  ( $Record_Length_1, $Time, $Nb_Pts_Total, @Data[1..$Nb_Pts],
    $Record_Length_2 ) = unpack ( $Format, $Bytes );
#
# [...]
```

10.2 Decrypting the nucleation message.

When a nucleation occurs at run-time, MICRESS® issues a message summarising some information: the nucleation time, temperature at the bottom and undercooling are deemed to be self-explaining. First of all the "seed number" is printed: it sums up all the seeds which have been set (without consideration of the seed type). It also specifies 'where' this seed was set, i.e.: in a user-defined region, in the bulk, at a binary interface, a triple-junction, or higher-order one (quadruple point), as well as the phase of this seed. These two specifics are actually implicit knowing the seed type which is also specified. The final bit is the grain number which might require some explanations: it is a grain identifier which is used to formally assign each grain its own phase-field parameter: this number can be re-used, which means that if a grain disappears, its number might be re-used for a fresh nucleus.

MICRESS on-screen output

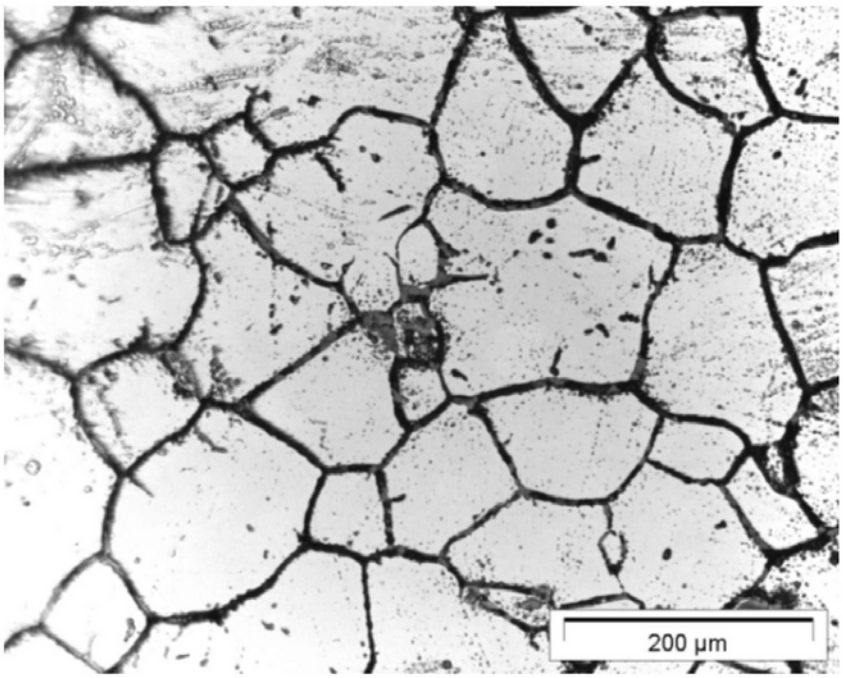
```
...
Seed number 5 set at time t = 1.00E-01 s
 -----------------------------------------------
 at a triple-junction
 Phase: 2
 Seed type: 1
 Temperature at the bottom = 1099.0 K
 Undercooling = 50.900 K
 Grain number = 14
...
```

10.3 Reading-in initial microstructures.

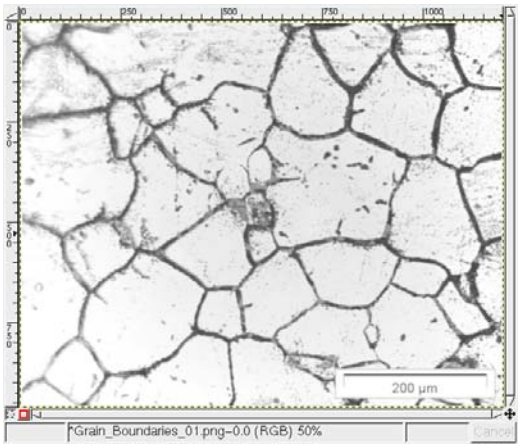
MICRESS® can read initial microstructure and composition or temperature fields from a file, to start from arbitrary initial conditions. The file to be read should be in ASCII with a know 'geometry' (number of cells in 'X' and 'Y' direction): the dimension of the read-in data set does not need to be identical to the simulation's. The most intricate case is probably reading an experimental grain structure, but this is not as daunting as it could seem.

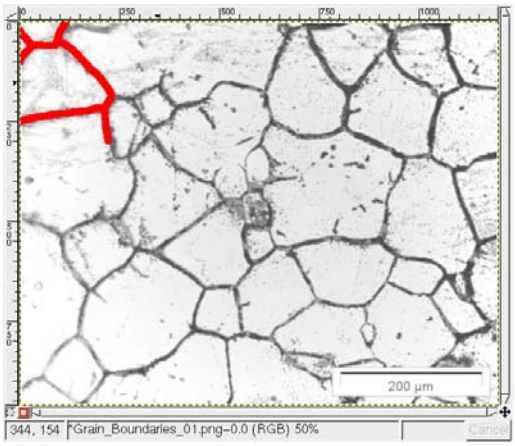
Here is a description of how it can be done with GIMP (GNU Image Manipulation Program), Version 1.2.5 (cf. www.gimp.org): newer versions have similar functionalities, but the naming might be slightly different. Any full-fledged image manipulation program should support similar procedures.

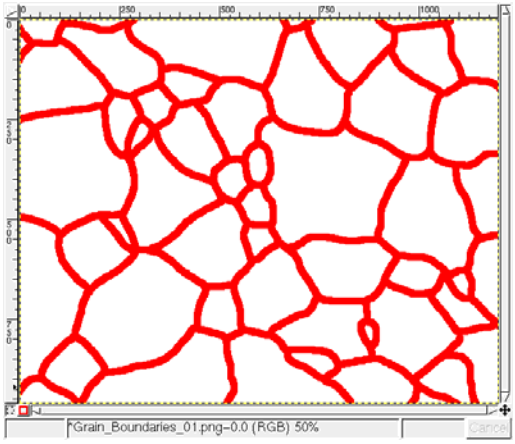
The initial micrograph is courtesy of IEHK, RWTH Aachen.



10.3.1 Step-by-step description.







1. Image/Transform/Zealous Crop/ to get rid of any frame.

2. Layers/Layers, Channels & Paths/Layers/: insert a new (transparent) layer.

3. Select a clearly different 'foreground color' (just to help see what has been drawn...).

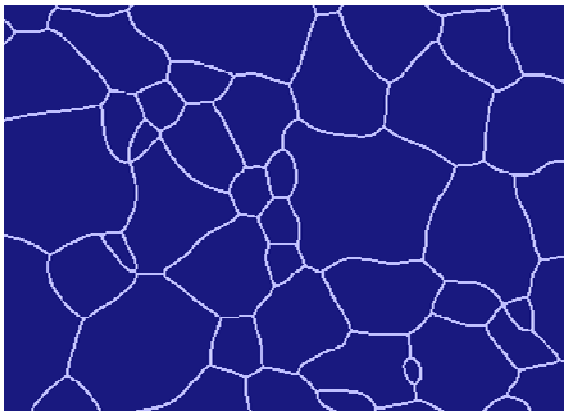
4. Tools/Paint Tools/Pencil to draw the boundaries on the transparent layer.

5. Layers/Layers, Channels & Paths/Layers/: remove the 'background' layer (original image) Make sure not to leave 'dangling' boundaries, so that each grain is ‘closed’ (the boundaries of the domain themselves do not have to be re-drawn, as MICRESS will perform this task, see note on the boundary conditions hereafter).

6. Image/Mode/Indexed: Use Black/White (1-Bit) Palette, No Color Dithering.

7. File/Save as/ save to ".pgm", by ‘Exporting’ first (make sure to save the file in ASCII).

8. This file has to be somewhat massaged into a shape fit for MICRESS consumption, please see the note on this topic hereafter.



It is probably not the best solution, certainly not even the easiest one, but it's relatively straightforward, not time-consuming, and... It works!

The “grain growth” standard examples provide an example of how such data can be then read by MICRESS®. Please also see the corresponding section in the description of the contents of a driving file, Read initial microstructure from a file.

10.3.2 Knocking a “pgm” file in shape.

The step ‘6’, switching to a 1-Bit palette, is slightly undone when saving as PGM (which stands for "Portable Gray Map"), as it is then exported as a level of greys map.

Furthermore somewhat outdated versions of Gimp (i.e., less than 2.0) actually saved PGMs with 3 RGB channels, requiring a script such as ‘*PGM_to_MICRESS*’ (available on request) to revert to the single value per pixel expected by MICRESS; newer versions of Gimp do save PGM as level of greys, therefore only requiring the header to be removed to make it a suitable input for MICRESS:

The first four lines of the output of an older GIMP:	The same for a ‘newer’ GIMP:
P3	*P2*
# CREATOR: The GIMP's PNM Filter Version 1.0	*# CREATOR: The GIMP's PNM Filter Version 1.0*
500 400	*500 400*
255	*255*
255	*255*

The key point is the first line: “P2” can simply be edited by hand: the header (i.e. the first four lines) can merely be deleted by hand with a text-editor, whereas “P3” also requires some further processing.

P2	'Magic number' for identifying the file type
# CREATOR: The GIMP's PNM Filter Version 1.0	Comment
500 400	Image width and height
255	Maximum grey value (Maxval)
255	Value for the first pixel:
	↳not the header anymore!

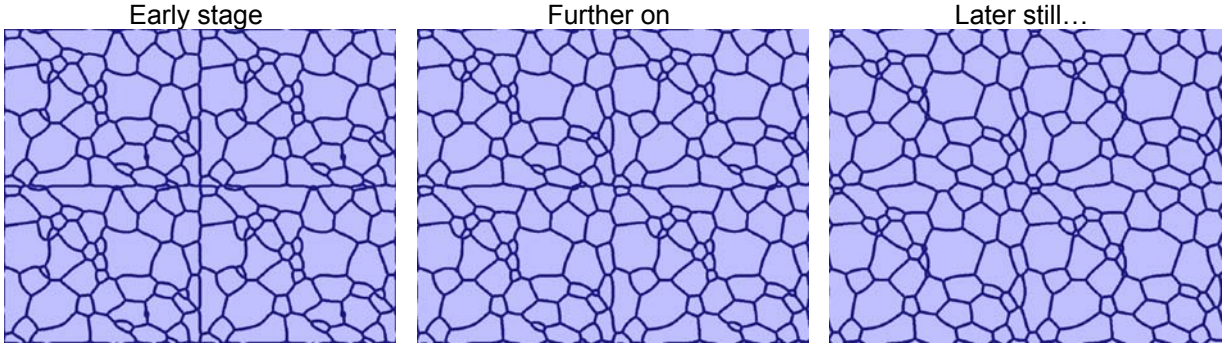
(Please remember that MICRESS will need the number of pixels in each direction).

10.3.3 Boundary conditions.

The readers who can still think creatively might have been wondering about the boundaries conditions: no need to worry, MICRESS will get it right!

First of all, grains touching the boundaries will be ‘closed’, so that they do not get merged with others. The user is also not restricted in any way in the choice of boundary conditions: even wrap-around, though initially leading to somewhat unexpected grain structures, subsequently allow proper relaxation. (See hereafter a four-folded symmetry view of the ‘Grain_Growth’ standard example).

Early stage | Further on | Later still…



11 Appendix.

11.1 Glossary.

Display_MICRESS	Post-processing tool performing a wide range of actions.
GrWin	Graphical library, which is used as a driver for the Windows version of *Display MICRESS*. (http:/spdg1.sci.shizuoka.ac.jp/grwinlib/english/).
GUI	Graphical User Interface, supports mouse actions.
PGPlot	Graphical library upon which DP_MICRESS is layered. (http://www.astro.caltech.edu/~tjp/pgplot).
Perl	Common scripting language, its Tk module provides most GUI features of Display MICRESS. For the ease of installation, it is 'packed' as standalone binary with PAR. (see respectively www.perl.org, www.ni-s.u-net.com, and par.perl.org).
PNG	Format for image output of DP_MICRESS, these operations are handled by the PNG library. *PNG* format is similar to *GIF* and widely supported by recent software, it has the distinctive advantage of being open-source, and actually happens to be more efficient than *GIF*. (www.libpng.org).
Transfer_MICRESS	Tool to convert MICRESS results files (bundled with DP_MICRESS).
Zlib	Compression library used for (de-)compressing files in MICRESS and DP_MICRESS , as well as for writing PNG images (from Display_MICRESS). (www.zlib.net).

11.2 Reference list.

Please note that an up-to-date list of publications (including links to some of the publications themselves) can be found at www.micress.de.

[1] A phase-field concept for multiphase systems, I. Steinbach, F. Pezzola, B. Nestler, M. Seeßelberg, R. Prieler, G.J. Schmitz, J.L.L. Rezende. In Physica D, 1996, pp. 135-147.

[2] The multiphase-field model with an integrated concept for modelling solute diffusion, J. Tiaden, B. Nestler, H.J. Diepers, I. Steinbach. In Physica D, 1998, pp. 73-86.

[3] Direct numerical simulation of solidification structure using the phase field method, I. Steinbach, G.J. Schmitz. In Modelling of Casting, Welding and Advanced Solidification Processes VIII.

[4] A generalized field method for multiphase transformations using interface fields, I. Steinbach, F. Pezzola. In Phzysica D, 1999, pp. 358-393.

[5] Multicomponent Multiphase Solidification of Ni-Base Superalloys: Phase Field Simulations Coupled to Thermodynamic Databases, U. Grafe, B. Bötger, J. Tiaden, S.G. Fries, I. Steinbach. In Modelling of Casting, Welding and Advanced Solidification Processes IX.

[6] Dual Scale Simulation of Grain Growth Using a Multi Phase Field Model, I. Steinbach, M. Apel. To be published in Proceedings of MRS Spring Conference 2001, Symp. AA.

[7] Simulation of Grain-Growth Using the Multi-Phase Field Method, I. Steinbach, M. Apel, P. Schaffnit. To be published in Proceedings of ReXPGG.

[8] Simulation of the γ-α-transformation using the phase-field method, Pariser, G.; Schaffnit, P.; Steinbach, I.; Bleck, W. In Steel Research 72(2001) No.9, p.354/60.

[9] History effects during the selection of primary dendrite spacing. Comparison of phase-field simulations with experimental observations, H.-J. Diepers, D. Ma, I. Steinbach. In Journal of Crystal Growth 237-239 (2002), p. 149-153.

[10] 2D and 3D phase-field simulations of lamellar and fibrous eutectic growth, M. Apel, B. Böttger, H.-J. Diepers, I. Steinbach. Journal of Crystal Growth 237-239 (2002) p.154-158.

[11] Simulation of Proeutectoid Ferrite Precipitation during Technical Heat Treatment, Pariser, G.; Schaffnit, P.; Steinbach, I.; Bleck, W. In MS&T 2003 Austenite Formation and Decomposition, E.B. Damm, M.J. Erwin (edt.), 9.-12. November 2003, Chicago, p. 279/290.

[12] Analysis of the gamma-alpha Transformation in C-Mn steel by phase-field modelling, M.G. Mecozzi, J.Sietsma, S.van der Zwaag, M.Apel, P.Schaffnit, I.Steinbach. In Metallurgical and Materials Transactions A 36A 9 (2005) 2327.

[13] Transient growth and interaction of equiaxed dendrites, I. Steinbach, HJ Diepers, C Beckermann. In Journal of Crystal Growth 275 3-4(2005) 624.

[14] An effective mobility approach to solute drag in computer simulations of migrating grain boundaries, H. Strandlund, J. Odqvist and J. Ågren. Submitted manuscript.

[15] Interaction of interdendritic convection and dendritic primary spacing: Phase-field simulation and analytical modelling, H.J. Diepers, I Steinbach. In SOLIDIFICATION AND GRAVITY IV, MATERIALS SCIENCE FORUM 508 (2006)145.

[16] Phase field simulation of equiaxed solidification in technical alloys, B. Boettger, J. Eiken, I. Steinbach. In Acta Materialia 54 10 (2006) 2697.

[17] Controlling Microstructure in Magnesium alloys: A combined thermodynamic, experimental and simulation approach, B. Boettger, J.Eiken, M.Ohno, G.Klaus, M.Fehlbier, R.Schmid-Fetzer, I.Steinbach and A. Bührig-Polaczek:. In Advanced Engineering Materials 8 4 (2006) 241.

[18] Multi Phase Field Model for Solid State Transformation with Elastic Strain, I.Steinbach, M.Apel. In Physica D 217 (2006) 153-160.

[19] Multiphase-Field approach for multicomponent alloys with extrapolation scheme for numerical application, J. Eiken , B.Boettger, I.Steinbach. In Phys. Rev. E 73 066122 (2006).

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a) PGPLOT Fortran Graphics Subroutine Library Version 5.2.2

Graphical library upon which DP_MICRESS is layered (www.astro.caltech.edu/~tjp/pgplot).

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```
*******************************************************************************
*                    PGPLOT Fortran Graphics Subroutine Library                *
*                                 Version 5.2.2                                *
*******************************************************************************

*******************************************************************************
*                                                                             *
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*          For further information, contact:                                  *
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*            105-24 California Institute of Technology,                       *
*            Pasadena, California 91125, USA                                  *
*                                                                             *
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```

b) libPNG

The object code of Display MICRESS has been created including source code from the PNG library. (www.libpng.org/pub/png/pngcode.html).

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The Contributing Authors and Group 42, Inc. specifically permit, without fee, and encourage the use of this source code as a component to supporting the PNG file format in commercial products.

c) zlib

Compression library used in DP_MICRESS for writing PNG images and compressing files.

(www.info-zip.org/pub/infozip/zlib)

zlib.h -- interface of the 'zlib' general purpose compression library version 1.1.3, July 9th, 1998

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The data format used by the zlib library is described by RFCs (Request for Comments) 1950 to 1952 in the files ftp://ds.internic.net/rfc/rfc1950.txt (zlib format), rfc1951.txt (deflate format) and rfc1952.txt (gzip format).

d) GrWin

Graphical library, which is used as a driver for the Windows version of Display MICRESS

http://spdg1.sci.shizuoka.ac.jp/grwinlib/english/

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11.3.10 Severability.

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11.3.11 Integration.

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phone ++49 241 80 98000, Fax: +49 241 38578, email: support.micress@access.rwth-aachen.de

11.4 Driving file.

```
#
# Automatic 'Driving File' written out by MICRESS.
#
#
# Type of input?
# ==============
shell input
#
#
# MICRESS binary
# ==============
# version number: 5.307 (Linux)
# compiled: 05/10/2007
# ('single precision' binary)
# permanent license
#
#
# Language settings
# =================
#  Please select a language: 'English', 'Deutsch' or 'Francais'
English
#
#
# Flags and settings
# ==================
#
# Geometry
# --------
# Grid size?
# (for 2D calculations: AnzY=1, for 1D calculations: AnzX=1, AnzY=1)
# AnzX:
250
# AnzY:
1
# AnzZ:
250
# Cell dimension (grid spacing in micrometers):
0.25000000
#
# Flags
# -----
# Type of coupling?
# Options:     phase  concentration  temperature  temp_cyl_coord
#              [stress]  [stress_coupled]  [flow]
concentration
# Type of potential?
# Options:     double_obstacle     double_well
double_obstacle
# Enable averaging of the driving force along the normal to the interface?
# Options:     averaging     no_averaging
averaging
# Enable one dimensional far field approximation for diffusion?
# Options:     1d_far_field    no_1d_far_field
no_1d_far_field
# Shall an additional 1D field be defined in z direction
# for temperature coupling?
# Options:     no_1d_temp  1d_temp  1d_temp_cylinder  1d_temp_polar
no_1d_temp
#
# Phase field data structure
# --------------------------
# Coefficient for initial dimension of field iFace
#  [minimum usage] [target usage]
0.1
# Coefficient for initial dimension of field nTupel
#  [minimum usage] [target usage]
0.1
```

```
# Restart options
# ===============
# Restart using old results?
# Options:    new       restart
new
#
#
# Name of output files
# ====================
# Name of result files?
Results_Gamma_Alpha/Gamma_Alpha
# Overwrite files with the same name?
# Options:    overwrite      write_protected     append
#             [zipped|not_zipped]                [unix|windows|non_native]
overwrite
#
#
# Selection of the outputs
# ========================
# Restart data output?                                  ('rest')
# Options:     out_restart      no_out_restart          [wallclock time, h.]
out_restart
# Grain number output?                                  ('korn')
# Options:     out_grains       no_out_grains
out_grains
# Phase number output?                                  ('phas')
# Options:     out_phases       no_out_phases           [no_interfaces]
out_phases
# Fraction output?                                      ('frac')
# Options:     out_fraction     no_out_fraction         [phase number]
no_out_fraction
# Average fraction table?                               ('TabF')
# Options:     tab_fractions    no_tab_fractions        [front_temperature]
tab_fractions
# Interface output?                                     ('intf')
# Options:     out_interface    no_out_interface        [sharp]
out_interface
# Driving-force output?                                 ('driv')
# Options:     out_driv_force   no_out_driv_force
out_driv_force
# Interface mobility output?                            ('mueS')
# Options:     out_mobility     no_out_mobility
no_out_mobility
# Curvature output?                                     ('krum')
# Options:     out_curvature    no_out_curvature
no_out_curvature
# Interface velocity output?                            ('vel')
# Options:     out_velocity     no_out_velocity
no_out_velocity
# Should the grain-time file be written out?            ('TabK')
# Options:     tab_grains       no_tab_grains           [extra|standard]
tab_grains
# Should the 'von Neumann Mullins' output be written out?       ('TabN')
# Options:    tab_vnm    no_tab_vnm
no_tab_vnm
# Should the 'grain data output' be written out?        ('TabGD')
# Options:    tab_grain_data    no_tab_grain_data
no_tab_grain_data
# Temperature output?                                   ('temp')
# Options:     out_temp         no_out_temp
no_out_temp
# Concentration output?                                 ('conc')
# Options:     out_conc         no_out_conc             [list of comp.]
out_conc
# Concentration of reference phase output?              ('cPha')
# Options:     out_conc_phase   no_out_conc_phase       [phase nb.] [l. of comp.]
no_out_conc_phase
# Average concentration per phase (and extrema)?        ('TabC')
# Options:     tab_conc       no_tab_conc
no_tab_conc
# Recrystallisation output?                             ('rex')
# Options:     out_recrystall   no_out_recrystall
no_out_recrystall
```

```
# Recrystallysed fraction output?                        ('TabR')
# Options:     tab_recrystall   no_tab_recrystall
no_tab_recrystall
# Miller-Indices output?                                 ('mill')
# Options:     out_miller       no_out_miller
no_out_miller
# Orientation output?                                    ('orie')
# Options:     out_orientation  no_out_orientation
no_out_orientation
# Should the orientation-time file be written out?       ('TabO')
# Options:     tab_orientation  no_tab_orientation
no_tab_orientation
# Should monitoring outputs be written out?              ('TabL')
# Options:     tab_log [simulation time, s] [wallclock time, min]  no_tab_log
tab_log 0.25
#
#
# Time input data
# ===============
# Finish input of output times (in seconds) with 'end_of_simulation'
# 'regularly-spaced' outputs can be set with 'linear_step'
# or 'logarithmic_step' and then specifying the increment
# and end value
00.25
01.00
linear_step 00.50 10.00
linear_step 01.00 25.00
end_of_simulation
# Time-step?
# Options:  (real)   automatic [0<factor_1<=1] [0<=factor_2] [max.] [min.]
# (Fix time steps: just input the value)
automatic
# Coefficient for phase-field criterion 1.00
# Coefficient for segregation criterion 1.00
# Number of iterations for initialisation?
25
#
#
# Phase data
# ==========
# Number of distinct solid phases?
2
#
# Data for phase 1:
# -----------------
# Simulation of recrystallisation in phase 1 ?
# Options:   recrystall     no_recrystall
no_recrystall
# Is phase 1 anisotrop?
# Options:   isotropic   anisotropic    faceted
isotropic
# Should grains of phase 1 be reduced to categories?
# Options:   categorize no_categorize
no_categorize
#
# Data for phase 2:
# -----------------
# Simulation of recrystallisation in phase 2 ?
# Options:   recrystall     no_recrystall
no_recrystall
# Is phase 2 anisotrop?
# Options:   isotropic   anisotropic    faceted
isotropic
# Should grains of phase 2 be reduced to categories?
# Options:   categorize no_categorize
no_categorize
```

```
# Grain input
# ===========
# Type of grain positioning ?
# Options:  deterministic   random   from_file
deterministic
# Number of grains at the beginning?
9
# Input data for grain number 1:
# Geometry?
# Options:  round     rectangular    elliptic
round
# x,z coordinates [micrometers], grain number 1?
51.240002
20.969999
# Grain radius?   [micrometers]
23.360001
# Shall grain 1 be stabilized or shall
# an analytical curvature description be applied?
# Options:    stabilisation   analytical_curvature
stabilisation
# Voronoi criterion?
# Options:    voronoi     no_voronoi
voronoi
# Phase number?   (integer)
1
# Input data for grain number 2:
# Geometry?
# Options:  round     rectangular    elliptic
round
# x,z coordinates [micrometers], grain number 2?
52.099998
47.365002
# Grain radius?   [micrometers]
25.860001
# Shall grain 2 be stabilized or shall
# an analytical curvature description be applied?
# Options:    stabilisation   analytical_curvature
stabilisation
# Voronoi criterion?
# Options:    voronoi     no_voronoi
voronoi
# Phase number?   (integer)
1
# Input data for grain number 3:
# Geometry?
# Options:  round     rectangular    elliptic
round
# x,z coordinates [micrometers], grain number 3?
37.130001
23.030001
# Grain radius?   [micrometers]
23.809999
# Shall grain 3 be stabilized or shall
# an analytical curvature description be applied?
# Options:    stabilisation   analytical_curvature
stabilisation
# Voronoi criterion?
# Options:    voronoi     no_voronoi
voronoi
# Phase number?   (integer)
1
```

```
# Input data for grain number 4:
# Geometry?
# Options:  round     rectangular    elliptic
round
# x,z coordinates [micrometers], grain number 4?
3.2449999
21.129999
# Grain radius?   [micrometers]
23.870001
# Shall grain 4 be stabilized or shall
# an analytical curvature description be applied?
# Options:    stabilisation   analytical_curvature
stabilisation
# Voronoi criterion?
# Options:    voronoi     no_voronoi
voronoi
# Phase number?   (integer)
1
# Input data for grain number 5:
# Geometry?
# Options:  round     rectangular    elliptic
round
# x,z coordinates [micrometers], grain number 5?
13.170000
35.485001
# Grain radius?   [micrometers]
27.020000
# Shall grain 5 be stabilized or shall
# an analytical curvature description be applied?
# Options:    stabilisation   analytical_curvature
stabilisation
# Voronoi criterion?
# Options:    voronoi     no_voronoi
voronoi
# Phase number?   (integer)
1
# Input data for grain number 6:
# Geometry?
# Options:  round     rectangular    elliptic
round
# x,z coordinates [micrometers], grain number 6?
29.305000
12.820000
# Grain radius?   [micrometers]
27.770000
# Shall grain 6 be stabilized or shall
# an analytical curvature description be applied?
# Options:    stabilisation   analytical_curvature
stabilisation
# Voronoi criterion?
# Options:    voronoi     no_voronoi
voronoi
# Phase number?   (integer)
1
# Input data for grain number 7:
# Geometry?
# Options:  round     rectangular    elliptic
round
# x,z coordinates [micrometers], grain number 7?
4.7849998
31.465000
# Grain radius?   [micrometers]
25.370001
# Shall grain 7 be stabilized or shall
# an analytical curvature description be applied?
# Options:    stabilisation   analytical_curvature
stabilisation
# Voronoi criterion?
# Options:    voronoi     no_voronoi
voronoi
# Phase number?   (integer)
1
```

```
# Input data for grain number 8:
# Geometry?
# Options:  round     rectangular    elliptic
round
# x,z coordinates [micrometers], grain number 8?
2.1550000
2.4900000
# Grain radius?   [micrometers]
27.945000
# Shall grain 8 be stabilized or shall
# an analytical curvature description be applied?
# Options:    stabilisation   analytical_curvature
stabilisation
# Voronoi criterion?
# Options:    voronoi     no_voronoi
voronoi
# Phase number?   (integer)
1
# Input data for grain number 9:
# Geometry?
# Options:  round     rectangular    elliptic
round
# x,z coordinates [micrometers], grain number 9?
42.174999
4.6100001
# Grain radius?   [micrometers]
24.150000
# Shall grain 9 be stabilized or shall
# an analytical curvature description be applied?
# Options:    stabilisation   analytical_curvature
stabilisation
# Voronoi criterion?
# Options:    voronoi     no_voronoi
voronoi
# Phase number?   (integer)
1
#
#
# Data for further nucleation
# ===========================
# Enable further nucleation?
# Options:     nucleation       no_nucleation
nucleation
# Additional output for nucleation?
# Options:     out_nucleation     no_out_nucleation
no_out_nucleation
#
# Data for further nucleation
# ---------------------------
# Number of types of seeds?
3
#
```

```
# Input for seed type 1:
# ----------------------
# Type of 'position' of the seeds?
# Options:   bulk   region   interface   triple   quadruple   [restrictive]
triple
# Phase of new grains?
2
# Reference phase?
1
# maximum number of new nuclei 1?
250
# Grain radius [micrometers]?
0.0000
# Choice of growth mode:
# Options:   stabilisation analytical_curvature
stabilisation
# min. undercooling [K] (>0)?
50.000
# Shield effect:
# Shield time [s] ?
20.000
# Shield distance [micrometers]?
2.5000
# Nucleation range
# min. nucleation temperature for seed type 1 [K]
1000.0
# max. nucleation temperature for seed type 1 [K]
1200.0
# Time between checks for nucleation? [s]
1E-1
# Shall random noise be applied?
# Options:     nucleation_noise   no_nucleation_noise
no_nucleation_noise
#
# Input for seed type 2:
# ----------------------
# Type of 'position' of the seeds?
# Options:   bulk   region   interface   triple   quadruple   [restrictive]
interface
# Phase of new grains?
2
# Reference phase?
1
# Substrat phase?
# (for taking into account curvature undercooling, set to 1 to disable)
1
# maximum number of new nuclei 2?
500
# Grain radius [micrometers]?
0.0000
# Choice of growth mode:
# Options:   stabilisation analytical_curvature
stabilisation
# min. undercooling [K] (>0)?
55.000
# Shield effect:
# Shield time [s] ?
20.000
# Shield distance [micrometers]?
2.5000
# Nucleation range
# min. nucleation temperature for seed type 2 [K]
1000.0
# max. nucleation temperature for seed type 2 [K]
1200.0
# Time between checks for nucleation? [s]
1E-1
# Shall random noise be applied?
# Options:     nucleation_noise   no_nucleation_noise
no_nucleation_noise
```

```
# Input for seed type 3:
# ----------------------
# Type of 'position' of the seeds?
# Options:   bulk   region   interface   triple   quadruple   [restrictive]
bulk
# Phase of new grains?
2
# Reference phase?
1
# Which nucleation model shall be used?
# Options:    seed_undercooling    seed_density
seed_undercooling
# maximum number of new nuclei 3?
500
# Grain radius [micrometers]?
0.0000
# Choice of growth mode:
# Options:   stabilisation analytical_curvature
stabilisation
# min. undercooling [K] (>0)?
65.000
# Shield effect:
# Shield time [s] ?
20.000
# Shield distance [micrometers]?
7.5000
# Nucleation range
# min. nucleation temperature for seed type 3 [K]
1000.0
# max. nucleation temperature for seed type 3 [K]
1200.0
# Time between checks for nucleation? [s]
1E-1
# Shall random noise be applied?
# Options:     nucleation_noise   no_nucleation_noise
no_nucleation_noise
#
# Max. number of simultaneous nucleations?
# ----------------------------------------
# (set to 0 for automatic)
0
#
# Shall metastable small seeds be killed?
# ---------------------------------------
# Options:     kill_metastable      no_kill_metastable
no_kill_metastable
#
#
# Phase interaction data
# ======================
#
# Data for phase interaction 0 / 1:
# ---------------------------------
# Simulation of interaction between phase 0 and 1 ?
# Options:   phase_interaction    no_phase_interaction
#            [standard|particle_pinning|solute_drag]
no_phase_interaction
#
# Data for phase interaction 0 / 2:
# ---------------------------------
# Simulation of interaction between phase 0 and 2 ?
# Options:   phase_interaction    no_phase_interaction
#            [standard|particle_pinning|solute_drag]
no_phase_interaction
```

```
# Data for phase interaction 1 / 1:
# --------------------------------
# Simulation of interaction between phase 1 and 1 ?
# Options:   phase_interaction    no_phase_interaction
#            [standard|particle_pinning|solute_drag]
phase_interaction
# Type of surface energy definition between phases 1 and 1?
# Options:  constant  temp_dependent
constant
# Surface energy between phases 1 and 1? [J/cm**2]
1.00000E-05
# Type of mobility definition between phases 1 and 1?
# Options:  constant  temp_dependent  sd_kth   dg_dependent
constant
# Kinetic coefficient mu between phases 1 and 1? [cm**4/(Js)]
1.00000E-05
#
# Data for phase interaction 1 / 2:
# --------------------------------
# Simulation of interaction between phase 1 and 2 ?
# Options:   phase_interaction    no_phase_interaction
#            [standard|particle_pinning|solute_drag]
phase_interaction
# 'DeltaG' options:  default
#                    avg ... []   max ... [J/cm**3]   smooth ... [degrees]
avg 1.   max 50.
# I.e.:  avg +1.00  smooth +45.0  max +5.00000E+01
# Type of surface energy definition between phases 1 and 2?
# Options:  constant  temp_dependent
constant
# Surface energy between phases 1 and 2? [J/cm**2]
5.00000E-05
# Type of mobility definition between phases 1 and 2?
# Options:  constant  temp_dependent  sd_kth   dg_dependent
constant
# Kinetic coefficient mu between phases 1 and 2? [cm**4/(Js)]
1.00000E-06
#
# Data for phase interaction 2 / 2:
# --------------------------------
# Simulation of interaction between phase 2 and 2 ?
# Options:   phase_interaction    no_phase_interaction
#            [standard|particle_pinning|solute_drag]
phase_interaction
# Type of surface energy definition between phases 2 and 2?
# Options:  constant  temp_dependent
constant
# Surface energy between phases 2 and 2? [J/cm**2]
2.00000E-05
# Type of mobility definition between phases 2 and 2?
# Options:  constant  temp_dependent  sd_kth   dg_dependent
constant
# Kinetic coefficient mu between phases 2 and 2? [cm**4/(Js)]
1.00000E-05
#
#
# Concentration data
# ==================
# Number of dissolved constituents?   (int)
2
# Type of concentration?
# Options:     atom_percent    (at%)
#              weight_percent  (wt%)
weight_percent
```

```
# Options:   diff     no_diff     infinite     multi
#            database_global     database_local
#            [+b] for grain-boundary diffusion
# ('multi' can be followed by a string of "n", "d", "g", or "l",
#  to describe each contribution: respectively no diffusion,
#  user-defined diffusion coefficient, and 'global' or 'local'
#  value from database, the default is global values from database).
# How shall diffusion of component 1 in phase 0 be solved?
no_diff
# How shall diffusion of component 1 in phase 1 be solved?
diff
# Diff.-coefficient:
# Prefactor? (real) [cm**2/s]
0.23400
# Activation energy? (real) [J/mol]
1.47700E+05
# How shall diffusion of component 1 in phase 2 be solved?
diff
# Diff.-coefficient:
# Prefactor? (real) [cm**2/s]
0.12300
# Activation energy? (real) [J/mol]
98290.
# How shall diffusion of component 2 in phase 0 be solved?
no_diff
# How shall diffusion of component 2 in phase 1 be solved?
diff
# Diff.-coefficient:
# Prefactor? (real) [cm**2/s]
0.15900
# Activation energy? (real) [J/mol]
2.61600E+05
# How shall diffusion of component 2 in phase 2 be solved?
diff
# Diff.-coefficient:
# Prefactor? (real) [cm**2/s]
127.00
# Activation energy? (real) [J/mol]
2.70800E+05
#
#
# Phase diagram - input data
# ==========================
#
# List of phases and components which are stoichiometric:
#  phase and component(s) numbers
# End with 'no_more_stoichio' or 'no_stoichio'
no_stoichio
#
# Is a thermodynamic database to be used?
# Options: database   no_database
no_database
```

```
# Input of the phase diagram of phase 1  and phase 2:
# ---------------------------------------------------
# Temperature of reference point? [K]
1149.9000
# Entropy of fusion between phase 1  and 2  ? (real) [J/(cm**3 K)]
0.14900
# Input of the concentrations at reference point
# Concentration of component 1  in phase 1 ? [wt%]
0.32000E-02
# dissolved concentration in phase 2 ? [wt%]
0.15811E-03
# Concentration of component 2  in phase 1 ? [wt%]
0.17399
# dissolved concentration in phase 2 ? [wt%]
0.96288E-01
# Input of the slopes at reference point
# Slope m_iPh = dT/dC_iPh relative to component 1  ? [K/wt%]
-386.5673523
# Slope m_jPh = dT/dC_jPh relative to component 1  ? [K/wt%]
-8036.549805
# Slope m_iPh = dT/dC_iPh relative to component 2  ? [K/wt%]
-39.82677078
# Slope m_jPh = dT/dC_jPh relative to component 2  ? [K/wt%]
-73.34864807
#
#
# Initial concentrations
# ======================
# How shall initial concentrations be set?
# Options:  input  equilibrium  from_file     [phase number]
equilibrium 1
# Initial concentration of component 1 in phase 1 ? [wt%]
3.20000E-03
# Initial concentration of component 2 in phase 1 ? [wt%]
0.17400
#
#
# Parameters for latent heat and 1D temperature field
# ===================================================
# Simulate release of latent heat?
# Options:       lat_heat     lat_heat_3d [matrix phase]     no_lat_heat
no_lat_heat
#
#
# Boundary conditions
# ===================
# Type of temperature trend?
# Options:      linear      linear_from_file      sinus
linear
# Number of connecting points?    (integer)
0
# Initial temperature at the bottom?  (real)  [K]
1100.0000
# Temperature gradient in z-direction?  [K/cm]
0.0000000
# Cooling rate? [K/s]
-10.0000000
# Moving-frame system in z-direction?
# Options:      moving_frame      no_moving_frame
no_moving_frame
# Boundary conditions for phase field in each direction
# Options: i (insulation) s (symmetric) p (periodic/wrap-around) g (gradient)
#          f (fixed)
# Sequence: E W (N S, if 3D) B T borders
pppp
# Boundary conditions for phase field in each direction
# Options: i (insulation) s (symmetric) p (periodic/wrap-around) g (gradient)
#          f (fixed)
# Sequence: E W (N S, if 3D) B T borders
pppp
# Unit-cell model symmetric with respect to the x/y diagonal plane?
# Options:    unit_cell_symm   no_unit_cell_symm
no_unit_cell_symm
```

```
# Other numerical parameters
# ==========================
# Phase minimum?
1.00E-04
# Interface thickness (in cells)?
5.00
#
#
```